Supporting Information

Palladium-Catalyzed C8-H Alkoxycarbonylation of 1-Naphthylamines with Alkyl chloroformates

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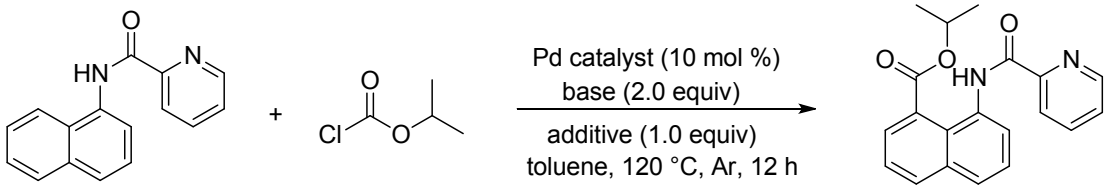
1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker DPX-400 spectrometer with $CDCl_3$ as the solvent and TMS as an internal standard. Melting points were measured using a WC-1 microscopic apparatus and are uncorrected. High resolution mass spectra were ensured on an Agilent Technologies 1290-6540 UHPLC/Accurate-Mass Quadrupole Time-of-Flight LC/MS. All solvents were used directly without further purification. Dichloromethane, ethyl acetate, and hexane were used for column chromatography. The commercials were obtained from commercial sources and used as-received without further purification unless otherwise noted.

2.Optimization of Reaction Conditions

Table S1. Optimization of Solvent and Catalyst[a]



1a **2a** **3aa**

Entry	catalyst	solvent	yield[b]
1	$Pd(OAc)_2$	DCE	0%
2	$Pd(OAc)_2$	CH_3CN	0%
3	$Pd(OAc)_2$	toluene	57%
4	$Pd(OAc)_2$	DMSO	0%
5	$Pd(OAc)_2$	1,4-dioxane	0%
6	$Pd(OAc)_2$	CH_3OH	0%
7	$Pd(OAc)_2$	DMF	0%
8	$Pd(OAc)_2$	actone	0%
9	$Cu(OAc)_2$	toluene	0%
10	$Co(OAc)_2$	toluene	0%
11	$NiCl_2$	toluene	0%
12	$FeCl_3$	toluene	0%
13	$RuCl_2$(*p*-cymene)$_2$	toluene	0%
14	$PdCl_2$	toluene	43%
15	$Pd(TFA)_2$	toluene	45%
16	$Pd(CH_3CN)_2Cl_2$	toluene	32%
17	Pd_2dba_3	toluene	0%
18	PdI_2	toluene	26%

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (3.0 equiv), catalysts (10 mol %), NaOAc (2.0 equiv) in solvent (1.0 mL) at 120 °C under argon for 12 h. [b] Isolated yield.

Table S2. Optimization of Base and Additive[a]

Entry	base	additive	yield [b]
1	$NaHCO_3$	-	18%
2	Na_2CO_3	-	40%
3	KOAc	-	75%
4	K_2CO_3	-	43%
5	Na_3PO_4	-	41%
6	Na_2HPO_4	-	35%
7	NaH_2PO_4	-	22%
8	PivONa	-	0%
9	Cs_2CO_3	-	0%
10	pyridine	-	0%
11	DBU	-	0%
12	NEt_3	-	0%
13	^{t}BuONa	-	47%
14	EtONa	-	44%
15	NaOAc	I_2	0%
16	NaOAc	NaI	81%
17	NaOAc	KI	73%
18	NaOAc	$AgSbF_6$	16%
19[c]	NaOAc	NaI	68%
20[d]	NaOAc	NaI	72%
21[e]	NaOAc	NaI	88%
19[e,f]	NaOAc	NaI	48%
20[e,g]	NaOAc	NaI	77%

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (3.0 equiv), $Pd(OAc)_2$ (10 mol %), base (2.0 equiv) and additive (1.0 equiv) in toluene (1.0 mL) at 120 °C under argon for 12 h. [b] Isolated yield. [c]At a additive loading of 30 mol %. [d]At a additive loading of 50 mol %. [e] $Pd(OAc)_2$ (15 mol %). [f] At 100 °C. [g] Under air.

3. Experimental Section

3.1. Typical procedure for the synthesis of substrate 1a

A 100 mL two-necked round-bottom flask was equipped with a magnetic stir bar and charged with 1-naphthylamine (20 mmol, 2.86 g), picolinic acid (1.1 equiv, 2.70 g), N,N-dimethyl-4-aminopyridine (DMAP, 0.1 equiv, 0.244 g) in 30 mL anhydrous CH_2Cl_2 at 0 ^{o}C. After EDCI (4.20 g, 1.1 equiv) in CH_2Cl_2 (20 mL) was added dropwise to the solution under a nitrogen atmosphere, the reaction was then warmed to room temperature, stirred for 12 h and quenched with water (30 mL). The reaction mixture was extracted with CH_2Cl_2 (3 × 20 mL), and the combined organic

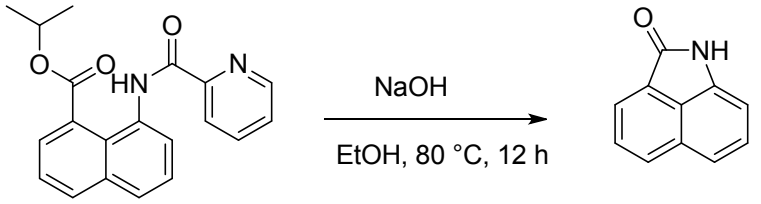
solvent was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The resulting residue was purified by column chromatography (hexane/ethyl acetate = 3:1) (V/V) to afford the pure product **1a** as a white solid (4.42 g, 89%).

All amides were prepared from the corresponding 1-naphthylamine derivatives and 2-picolinic acid according to the reported procedure.[1]

3.2. Typical procedure for the product 3aa

A Schlenk tube was equipped with a magnetic stir bar and charged with N-(naphthalen-1-yl)picolinamide **1a** (0.1 mmol, 24.8 mg), **2a** (0.3 mmol, 41 μL), NaOAc (0.2 mmol, 16 mg), $Pd(OAc)_2$ (0.015 mmol, 3.3 mg), NaI (0.1 mmol, 15 mg) in toluene (1.0 mL). The resulting mixture was sealed under argon, heated at 120 °C for 12 h, and cooled to room temperature. Upon completion, CH_2Cl_2 (20 mL) was added to the reaction system, and the resulting mixture was filtered through a pad of Celite. After the organic material was concentrated in vacuum, the product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (5:1, V/V) to afford the pure product **3aa**.

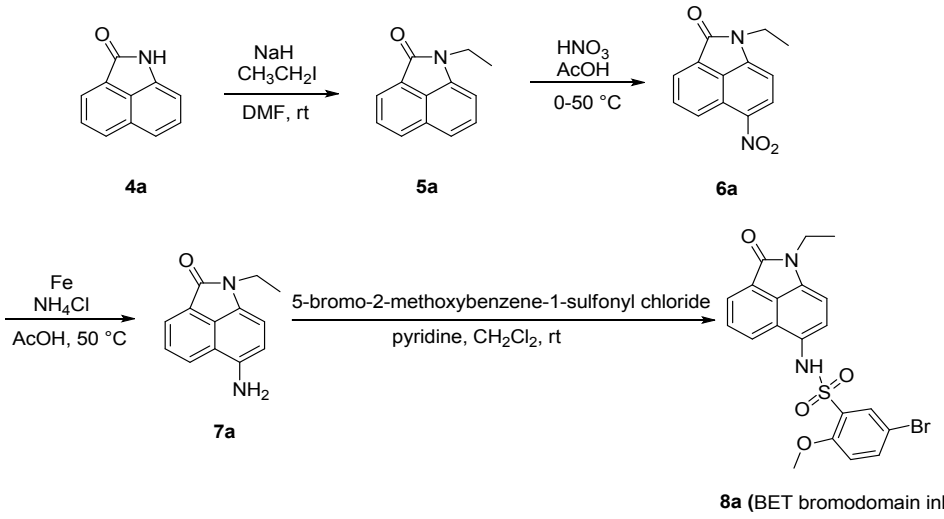
3.3. Typical procedure for the product 4a



3aa **4a** 55%

A mixture of **3aa** (66.8 mg, 0.2 mmol, 1.0 equiv) and NaOH (240 mg, 6 mmol, 30 equiv) was heated in ethanol (3.0 mL) for 12 h at 80 °C. After the mixture was cooled to room temperature and diluted with water (3.0 mL), the solution of diluted hydrochloric acid was added until it was acidic. The saturated $NaHCO_3$ solution was then added until the pH value was about 7. The mixture was then extracted with CH_2Cl_2 and dried over anhydrous Na_2SO_4. After the organic material was concentrated in vacuum, the product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (3:1, V/V) to afford the pure product **4a**.

3.4. Typical procedure for the product 8a



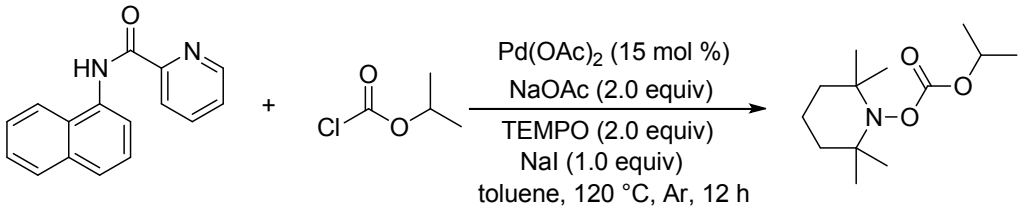
To a solution of **4a** (169 mg, 1.0 mmol, 1.0 equiv) in DMF (2.5 mL), NaH (36 mg, 1.5 mmol, 1.5 equiv) was added at 0 °C. After stirred for 10 min at 0 °C, iodoethane (96 μL, 1.2 mmol, 1.2 equiv) was added dropwise into the solution and the reaction mixture was stirred at room temperature. After the reaction was completed, the resulting mixture was poured into H_2O and extracted with ethyl acetate. The organic material was dried over Na_2SO_4 and concentrated in vacuum, and the product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (5:1, V/V) to afford the pure product **5a**.

To a solution of **5a** (189 mg, 0.96 mmol, 1.0 equiv) in AcOH (2.5 mL), HNO_3 (61 mg, 0.96 mmol, 1.0 equiv) was added at 0 °C and then the reaction mixture was stirred at 50 °C for 1 h. After the reaction was completed, the reaction mixture was cooled to room temperature. The mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4 and concentrated in vacuo, and the product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (5:1, V/V) to afford the pure product **6a**.

A mixture of iron powder (179 mg, 3.2 mmol, 5.0 equiv) and NH_4Cl (68 mg, 1.28 mmol, 2.0 equiv) in a mixture of AcOH/water (2 mL/8 mL) was heated at 50 °C for 5 min. Subsequently, **6a** (155 mg, 0.64 mmol, 1.0 equiv) was dissolved in DMF (2 mL) and added to the reaction mixture. After completion, the mixture was cooled to room temperature, extracted with ethyl acetate. After the organic layer was washed with brine, dried over Na_2SO_4 and filtered, the filtrate was concentrated in vacuo. The product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (3:1, V/V) to afford the pure product **7a**.

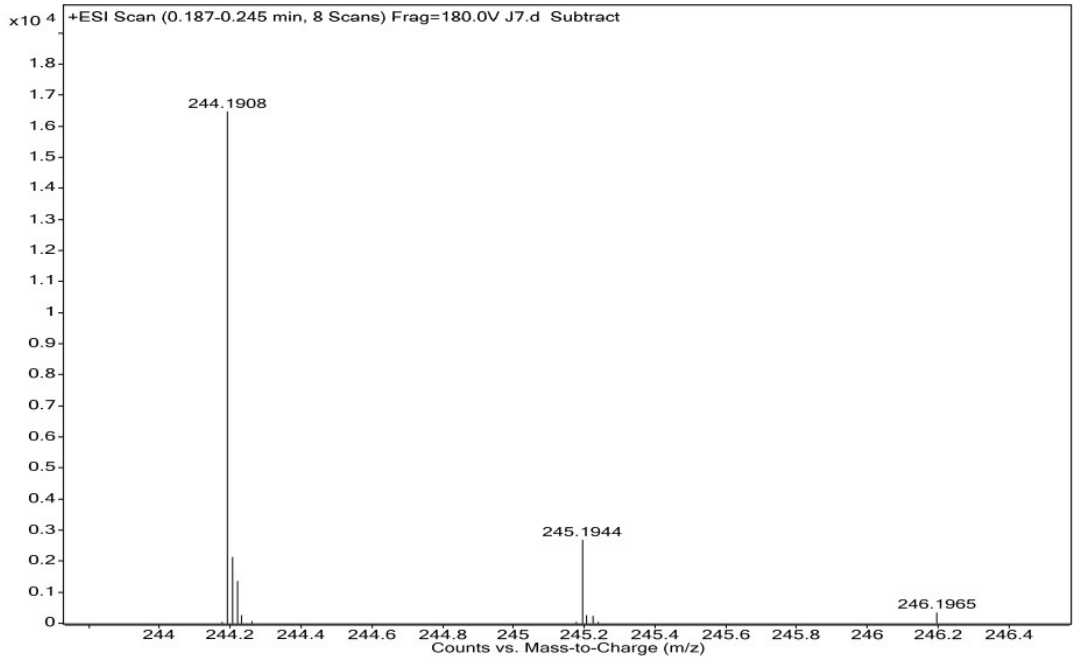
A mixture of **7a** (105 mg, 0.5 mmol, 1.0 equiv) and 5-bromo-2-methoxybenzenesulfonyl chloride (170 mg, 0.6 mmol, 1.2 equiv) in CH_2Cl_2 (10 mL) was added in pyridine (0.5 mL) and stirred at room temperature for 2 h. The mixture was extracted with CH_2Cl_2, and the organic layer was washed with brine, dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated in vacuo, and the product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (2:1, V/V) to afford the pure product **8a**.[2]

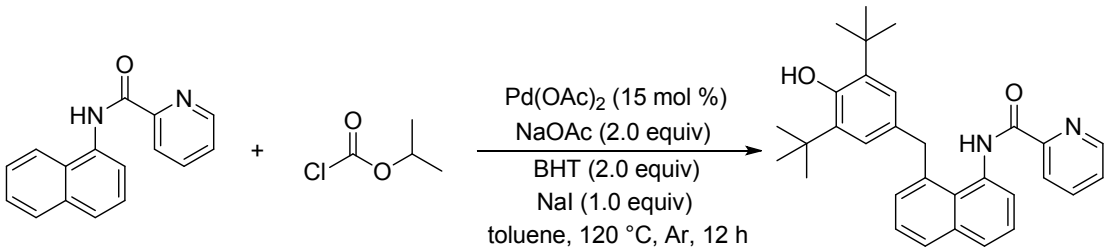
3.5. The experiment of trapping the radicals



1a **2a** **9a** *detected by HR-MS*

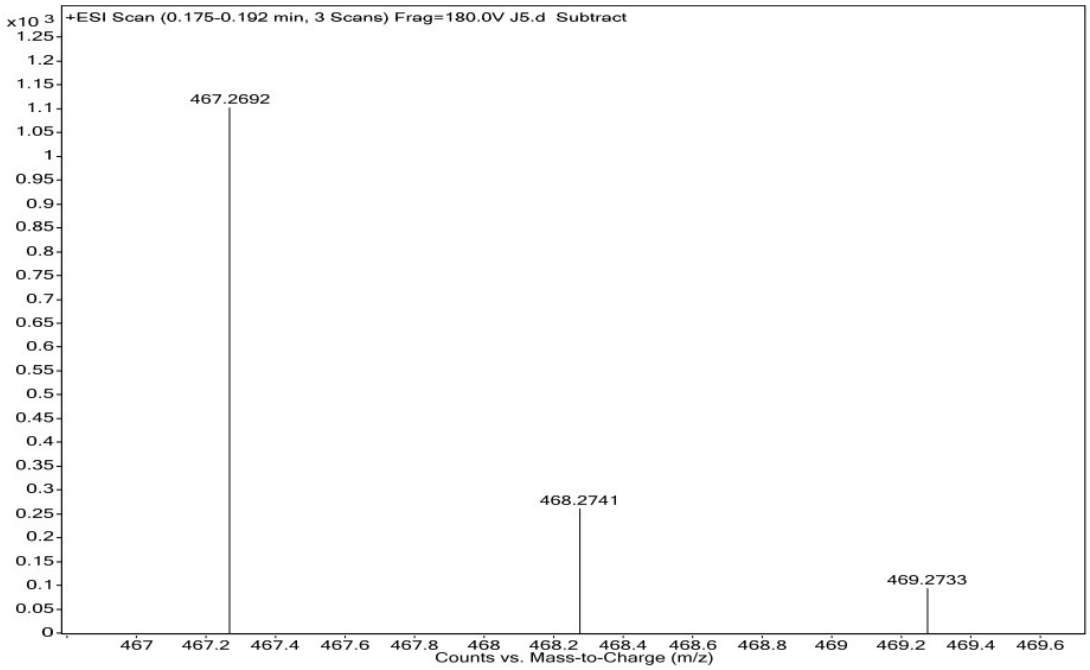
HRMS (ESI$^+$): calcd for $C_{13}H_{26}NO_3$ $[M+H]^+$: 244.1907, found: 244.1908.





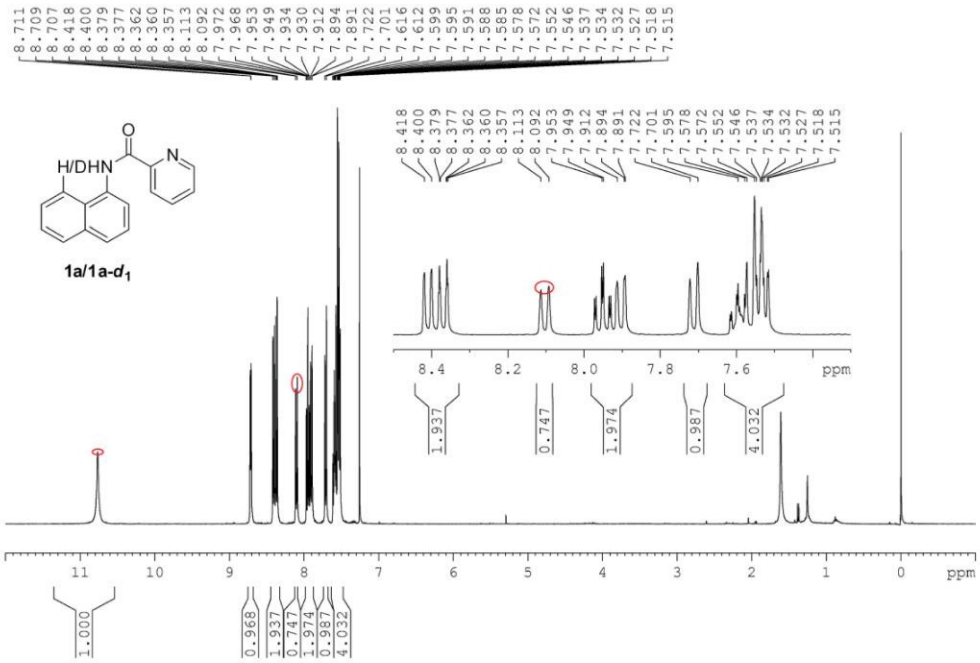
1a **2a** **10a** *detected by HR-MS*

HRMS (ESI$^+$): calcd for $C_{31}H_{35}N_2O_2$ $[M+H]^+$: 467.2693, found: 467.2692.

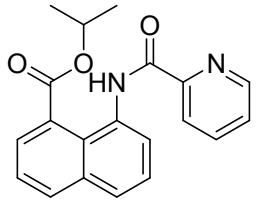


3.6. Kinetic isotope effect measurements

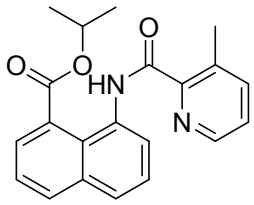
A Schlenk tube was equipped with a magnetic stir bar and charged with N-(naphthalen-1-yl)picolinamide **1a** (0.05 mmol, 12.4 mg), **1a-*d*$_1$** (0.05 mmol, 12.4 mg), **2a** (0.3 mmol, 41 μL), NaOAc (0.2 mmol, 16 mg), $Pd(OAc)_2$ (0.015 mmol, 3.3 mg), NaI (0.1 mmol, 15 mg) in toluene (1.0 mL). The resulting mixture was sealed under Ar, heated at 120 °C for 1 h and cooled to room temperature. Upon completion, CH_2Cl_2 (20 mL) was added to the reaction system, and the resulting mixture was filtered through a pad of Celite. After the organic material was concentrated in vacuum, the product was purified by column chromatography on silica gel (100–200 mesh) using hexane/EtOAc as an eluent (5:1, V/V) to afford the pure product **1a/1a-*d*$_1$**, and then analyzed by ^{1}H NMR spectrum. The KIE value was calculated as k_H/k_D = 0.3.



4. Characterization Data of the Products

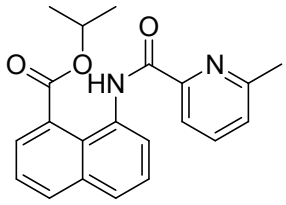


Isopropyl 8-(picolinamido)-1-naphthoate, **3aa**: yellow solid (29.4 mg, 88%); mp 110-112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.37 (s, 1H), 8.72-8.70 (m, 1H), 8.30-8.28 (m, 1H), 7.98 (dd, J_1 = 8.24 Hz, J_2 = 1.12 Hz, 1H), 7.92-7.88 (m, 2H), 7.84 (d, J = 7.20 Hz, 1H), 7.67-7.62 (m, 2H), 7.49-7.45 (m, 2H), 5.15-5.09 (m, 1H), 1.20 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 163.5, 150.2, 148.1, 137.5, 135.1, 131.9, 131.7, 129.4, 128.3, 127.5, 126.7, 126.5, 126.4, 125.7, 124.6, 122.8, 69.5, 21.6; HRMS (ESI$^+$): calcd for $C_{20}H_{19}N_2O_3$ $[M+H]^+$: 335.1390, found: 335.1391.

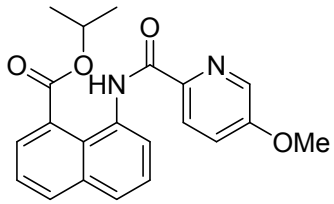


Isopropyl 8-(3-methylpicolinamido)-1-naphthoate, **3ba**: colorless solid (14.3 mg, 41%); mp 113-115 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 8.55 (dd, J_1 = 4.56 Hz, J_2 = 1.04 Hz, 1H), 7.97 (dd, J_1 = 8.24 Hz, J_2 = 1.12 Hz, 1H), 7.88-7.82 (m, 2H), 7.65-7.59 (m, 3H), 7.49-7.45 (m, 1H), 7.40-7.37 (m, 1H), 5.04-4.98 (m, 1H), 2.76 (s, 3H), 1.16 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100

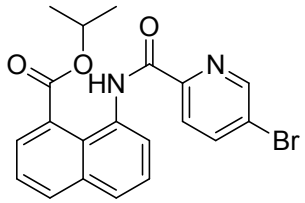
MHz, $CDCl_3$) δ 170.8, 165.1, 147.3, 145.5, 141.0, 136.2, 135.1, 132.1, 131.7, 130.0, 128.0, 127.3, 126.8, 126.3, 126.0, 124.5, 69.3, 21.5, 20.7; HRMS (ESI^+): calcd for $C_{21}H_{21}N_2O_3$, $[M+H]^+$: 349.1547, found: 349.1549.



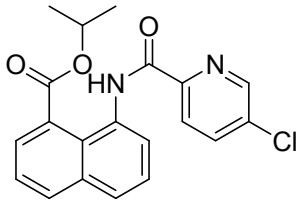
Isopropyl 8-(6-methylpicolinamido)-1-naphthoate, **3ca**: yellow solid (31.7 mg, 91%); mp 109-110 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 10.43 (s, 1H), 8.09 (d, J = 7.64 Hz, 1H), 7.97 (d, J = 8.08 Hz, 1H), 7.90 (d, J = 7.40 Hz, 1H), 7.83-7.75 (m, 2H), 7.65-7.58 (m, 2H), 7.46 (t, J = 7.62 Hz, 1H), 7.34 (d, J = 7.68 Hz, 1H), 5.09-5.02 (m, 1H), 2.70 (s, 3H), 1.13 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 163.8, 157.3, 149.4, 137.6, 135.1, 132.0, 129.5, 128.1, 127.4, 126.6, 126.4, 126.2, 125.8, 124.5, 119.8, 69.1, 24.1, 21.6; HRMS (ESI^+): calcd for $C_{21}H_{21}N_2O_3$ $[M+H]^+$: 349.1547, found: 349.1548.



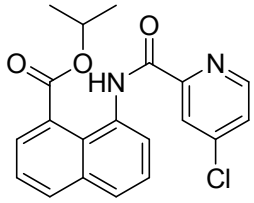
Isopropyl 8-(5-methoxypicolinamido)-1-naphthoate, **3da**: brown solid (28.8 mg, 79%); mp 76-79 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 8.36 (d, J = 2.80 Hz, 1H), 8.24 (d, J = 8.64 Hz, 1H), 7.90 (dd, J_1 = 8.24 Hz, J_2 = 1.12 Hz, 1H), 7.89 (d, J = 7.44, Hz, 1H), 7.83-7.81 (m, 1H), 7.66-7.58 (m, 2H), 7.48-7.45 (m, 1H), 7.33 (dd, J_1 = 8.68 Hz, J_2 = 2.84 Hz, 1H), 5.15-5.09 (m, 1H), 3.93 (s, 3H), 1.22 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 163.4, 158.1, 142.8, 136.4, 135.1, 131.9, 131.8, 129.5, 128.1, 127.3, 126.7, 126.4, 125.8, 124.5, 124.1, 120.3, 69.5, 55.8, 21.6; HRMS (ESI^+): calcd for $C_{21}H_{21}N_2O_4$ $[M+H]^+$: 365.1496, found: 365.1498.



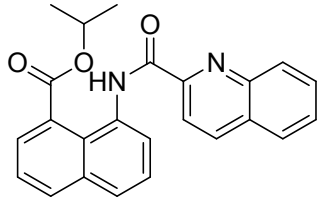
Isopropyl 8-(5-bromopicolinamido)-1-naphthoate, **3ea**: yellow solid (21.4 mg, 52%); mp 85-87 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.77 (dd, J_1 = 2.22 Hz, J_2 = 0.58 Hz, 1H), 8.18 (dd, J_1 = 8.32 Hz, J_2 = 0.56 Hz, 1H), 8.04 (dd, J_1 = 8.32 Hz, J_2 = 2.28 Hz, 1H), 7.99 (dd, J_1 = 8.24 Hz, J_2 = 1.12 Hz, 1H), 7.90 (d, J = 7.48 Hz, 1H), 7.84 (d, J = 8.16 Hz, 1H), 7.69 (dd, J_1 = 7.10 Hz, J_2 = 1.26 Hz, 1H), 7.61 (t, J = 7.84 Hz, 1H), 7.50-7.46 (m, 1H), 5.18-5.11 (m, 1H), 1.24 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 162.8, 149.2, 148.7, 140.2, 135.1, 132.1, 131.4, 129.2, 128.6, 127.7, 126.7, 126.3, 125.6, 124.6, 124.4, 124.3, 69.5, 21.6; HRMS (ESI^+): calcd for $C_{20}H_{18}BrN_2O_3$ $[M+H]^+$: 413.0495, found: 413.0497.



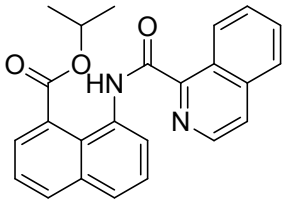
Isopropyl 8-(5-chloropicolinamido)-1-naphthoate, **3fa**: yellow solid (18.8 mg, 51%); mp 102-104 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.27 (s, 1H), 8.66 (d, J = 2.09 Hz, 1H), 8.25 (d, J = 8.27 Hz, 1H), 8.00 (dd, J_1 = 8.19 Hz, J_2 = 0.88 Hz, 1H), 7.91-7.84 (m, 3H), 7.69 (dd, J_1 = 7.11 Hz, J_2 = 1.26 Hz, 1H), 7.62 (t, J = 7.83 Hz, 1H), 7.50-7.46 (m, 1H), 5.18-5.11 (m, 1H), 1.24 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 162.6, 148.4, 147.1, 137.2, 135.4, 135.1, 132.1, 131.5, 129.2, 128.6, 127.7, 126.7, 126.3, 125.6, 124.6, 123.9, 69.5, 21.6; HRMS (ESI$^+$): calcd for $C_{20}H_{18}ClN_2O_3$ $[M+H]^+$: 369.1000, found: 369.0998.



Isopropyl 8-(4-chloropicolinamido)-1-naphthoate, **3ga**: white solid (28.3 mg, 77%); mp 146-148 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.35 (s, 1H), 8.61 (d, J = 5.24 Hz, 1H), 8.29 (d, J = 1.92 Hz, 1H), 8.00-7.98 (m, 1H), 7.91 (d, J = 7.44 Hz, 1H), 7.85 (d, J = 8.00 Hz, 1H), 7.70-7.68 (m, 1H), 7.62 (t, J = 7.82 Hz, 1H), 7.52-7.47 (m, 2H), 5.17-5.11 (m, 1H), 1.23 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 162.4, 151.7, 149.0, 146.0, 135.1, 132.2, 131.4, 129.1, 128.7, 127.7, 126.7, 126.4, 125.6, 124.6, 123.5, 69.5, 21.6; HRMS (ESI$^+$): calcd for $C_{20}H_{18}ClN_2O_3$ $[M+H]^+$: 369.1000, found: 369.1002.

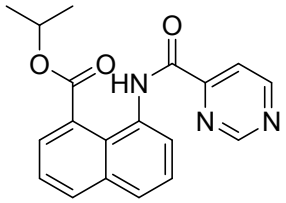


Isopropyl 8-(quinoline-2-carboxamido)-1-naphthoate, **3ha**: yellow solid (35.3 mg, 92%); mp 93-95 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.67 (s, 1H), 8.40-8.32 (m, 3H), 7.99-7.97 (m, 2H), 7.90 (dd, J_1 = 8.06 Hz, J_2 = 1.02 Hz, 1H), 7.84-7.79 (m, 2H), 7.68-7.60 (m, 3H), 7.49-7.45 (m, 1H), 5.09-5.03 (m, 1H), 1.01 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 163.7, 149.9, 146.5, 137.7, 135.2, 131.9, 130.3, 129.9, 129.5, 129.4, 128.3, 128.2, 127.8, 127.5, 126.6, 126.4, 125.8, 124.6, 119.1, 69.3, 21.5; HRMS (ESI$^+$): calcd for $C_{24}H_{21}N_2O_3$ $[M+H]^+$: 385.1547, found: 385.1548.

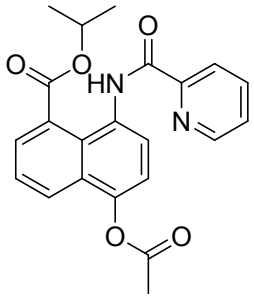


Isopropyl 8-(isoquinoline-1-carboxamido)-1-naphthoate, **3ia**: colorless solid (16.9 mg, 44%); mp 84-85 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 9.62-9.59 (m, 1H), 8.63 (d, J = 5.52 Hz,

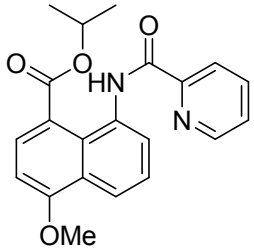
1H), 8.01-7.97 (m, 2H), 7.89-7.84 (m, 3H), 7.75-7.63 (m, 4H), 7.50-7.46 (m, 1H), 5.00-4.94 (m, 1H), 1.08 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 165.1, 148.2, 140.2, 137.5, 135.2, 132.0, 131.9, 130.6, 129.5, 128.9, 128.2, 127.8, 127.5, 127.3, 126.9, 126.8, 126.4, 125.9, 124.8, 124.6, 69.4, 21.5; HRMS (ESI$^+$): calcd for $C_{24}H_{21}N_2O_3$ $[M+H]^+$: 385.1547, found: 385.1548.



Isopropyl 8-(pyrimidine-4-carboxamido)-1-naphthoate, **3ja**: yellow oil (7.7 mg, 23%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.47 (s, 1H), 9.41 (d, J = 1.28 Hz, 1H), 9.04 (d, J = 5.00 Hz, 1H), 8.22 (dd, J_1 = 5.02 Hz, J_2 = 1.34 Hz, 1H), 8.02 (dd, J_1 = 8.22 Hz, J_2 = 1.06 Hz, 1H), 7.93 (d, J = 7.48 Hz, 1H), 7.87 (d, J = 8.08 Hz, 1H), 7.76 (dd, J_1 = 7.12 Hz, J_2 = 1.20 Hz, 1H), 7.63 (t, J = 7.84 Hz, 1H), 7.52-7.48 (m, 1H), 5.24-5.18 (m, 1H), 1.26 (d, J = 6.24 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 161.9, 159.4, 157.8, 156.8, 135.2, 132.5, 130.9, 129.2, 128.8, 128.1, 126.8, 126.3, 125.4, 124.7, 119.1, 69.7, 21.6; HRMS (ESI$^+$): calcd for $C_{19}H_{18}N_3O_3$ $[M+H]^+$: 336.1343, found: 336.1342.

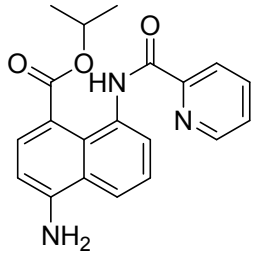


Isopropyl 5-acetoxy-8-(picolinamido)-1-naphthoate, **3ka**: brown oil (18.4 mg, 47%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.70 (d, J = 4.52 Hz, 1H), 8.29 (d, J = 7.76 Hz, 1H), 8.06-8.04 (m, 1H), 7.92-7.87 (m, 2H), 7.66 (d, J = 6.28 Hz, 1H), 7.54-7.49 (m, 2H), 7.41 (d, J = 8.20 Hz, 1H), 5.11-5.05 (m, 1H), 2.47 (s, 3H), 1.19 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 169.3, 163.6, 149.9, 148.1, 145.2, 137.5, 129.9, 129.7, 128.5, 128.2, 126.8, 126.6, 126.4, 125.2, 124.6, 122.9, 118.9, 69.7, 21.5, 21.1; HRMS (ESI$^+$): calcd for $C_{22}H_{21}N_2O_5$ $[M+H]^+$: 393.1445, found: 393.1444.

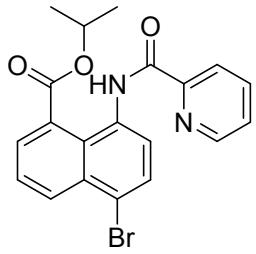


Isopropyl 4-methoxy-8-(picolinamido)-1-naphthoate, **3la**: brown solid (25.1 mg, 69%); mp 156-158 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.69 (d, J = 4.56 Hz, 1H), 8.31-8.26 (m, 2H), 7.96 (d, J = 7.32 Hz, 1H), 7.87 (t, = 7.70 Hz, 1H), 7.72 (d, J = 8.08 Hz, 1H), 7.61 (t, = 7.96 Hz,

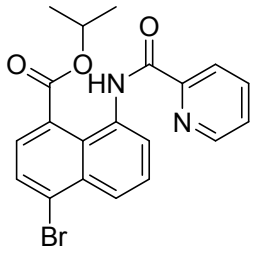
1H), 7.48-7.45 (m, 1H), 6.76 (d, J = 8.04 Hz, 1H), 5.19-5.12 (m, 1H), 4.00 (s, 3H), 1.21 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 163.5, 158.3, 150.3, 148.1, 137.4, 131.7, 130.4, 127.3, 127.2, 127.0, 126.4, 125.7, 122.8, 121.3, 121.1, 102.3, 69.1, 55.9, 21.6; HRMS (ESI^+): calcd for $C_{21}H_{21}N_2O_4$ $[M+H]^+$: 365.1496, found: 365.1499.



Isopropyl 4-amino-8-(picolinamido)-1-naphthoate, **3ma**: brown solid (13.3 mg, 38%); mp 130-133 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.78 (s, 1H), 8.72-8.71 (m, 1H), 8.43 (d, J = 7.48 Hz, 1H), 8.36 (d, J = 7.80 Hz, 1H), 8.00-7.89 (m, 3H), 7.74 (d, J = 8.56 Hz, 1H), 7.60-7.52 (m, 3H), 7.01 (s, 1H), 5.12-5.06 (m, 1H), 1.35 (d, J = 6.24 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.3, 154.0, 149.9, 148.2, 137.8, 133.5, 133.0, 127.0, 126.6, 126.2, 126.1, 122.5, 118.7, 117.3, 116.9, 69.1, 22.2; HRMS (ESI^+): calcd for $C_{20}H_{20}N_3O_3$ $[M+H]^+$: 350.1499, found: 350.1051.

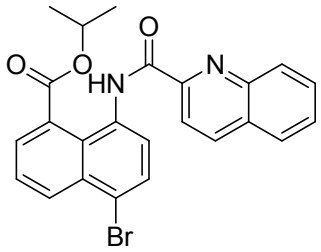


Isopropyl 5-bromo-8-(picolinamido)-1-naphthoate, **3na**: yellow solid (31.3 mg, 76%); mp 114-116 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 8.70 (d, J = 4.48 Hz, 1H), 8.45 (dd, J_1 = 8.52 Hz, J_2 = 1.00 Hz, 1H), 8.28 (d, = 7.84 Hz, 1H), 7.93-7.88 (m, 2H), 7.75 (d, J = 8.12 Hz, 1H), 7.68 (dd, J_1 = 7.04 Hz, J_2 = 1.12 Hz, 1H), 7.61-7.57 (m, 1H), 7.52-7.49 (m, 1H), 5.11-5.04 (m, 1H), 1.18 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 163.5, 149.8, 148.1, 137.6, 133.1, 131.7, 130.9, 130.6, 130.1, 128.8, 127.2, 127.0, 126.7, 126.1, 122.9, 121.6, 69.8, 21.5; HRMS (ESI^+): calcd for $C_{20}H_{18}BrN_2O_3$ $[M+H]^+$: 413.0495, found: 413.0496.

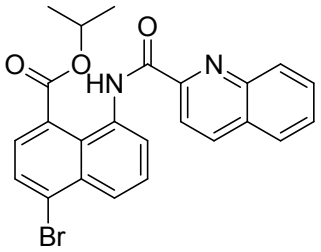


Isopropyl 4-bromo-8-(picolinamido)-1-naphthoate, **3oa**: yellow solid (28.4 mg, 69%); mp 114-116 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.27 (s, 1H), 8.71-8.69 (m, 1H), 8.34-8.28 (m, 2H), 7.93-7.88 (m, 2H), 7.80 (d, J = 7.68 Hz, 1H), 7.75-7.71 (m, 1H), 7.52-7.48 (m, 1H), 7.45 (d, J = 7.68 Hz, 1H), 5.07-5.01 (m, 1H), 1.17 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 163.6, 149.8, 148.1, 137.6, 133.4, 132.2, 129.6, 129.1, 127.9, 127.8, 127.7, 127.2, 126.8, 126.7, 126.6,

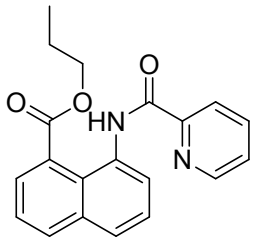
122.9, 69.8, 21.5; HRMS (ESI$^+$): calcd for $C_{20}H_{18}BrN_2O_3$ $[M+H]^+$: 413.0495, found: 413.0493.



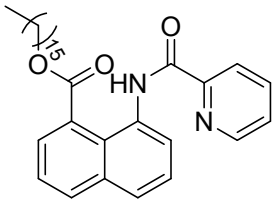
Isopropyl 5-bromo-8-(quinoline-2-carboxamido)-1-naphthoate, **3pa**: yellow solid (28.6 mg, 62%); mp 128-130 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.48 (dd, J_1 = 8.52 Hz, J_2 = 1.24 Hz, 1H), 8.38 (s, 2H), 8.33 (d, J = 8.44 Hz, 1H), 7.96-7.93 (m, 2H), 7.86-7.80 (m, 2H), 7.71-7.67 (m, 2H), 7.63-7.59 (m, 1H), 5.03-4.97 (m, 1H), 1.00 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 163.7, 149.5, 146.4, 137.8, 133.2, 131.9, 130.9, 130.6, 130.4, 130.2, 129.9, 129.5, 128.8, 128.3, 127.8, 127.3, 126.8, 126.1, 121.6, 119.0, 69.5, 21.0; HRMS (ESI$^+$): calcd for $C_{24}H_{20}N_2O_3$ $[M+H]^+$: 463.0652, found: 463.0653.



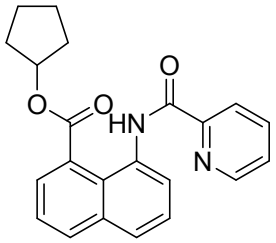
Isopropyl 4-bromo-8-(quinoline-2-carboxamido)-1-naphthoate, **3qa**: yellow solid (29.1 mg, 63%); mp 137-139 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.37-8.31 (m, 4H), 7.99 (d, J = 7.44 Hz, 1H), 7.93-7.91 (m, 1H), 7.85-7.80 (m, 2H), 7.75-7.71 (m, 1H), 7.69-7.65 (m, 1H), 7.46 (d, J = 7.68 Hz, 1H), 5.00-4.94 (m, 1H), 0.99 (d, J = 6.28 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 163.8, 149.6, 146.4, 137.7, 133.4, 132.3, 130.4, 129.9, 129.7, 129.5, 129.1, 128.3, 127.9, 127.8, 127.7, 127.6, 127.3, 126.8, 126.6, 119.1, 69.6, 21.4; HRMS (ESI$^+$): calcd for $C_{24}H_{20}N_2O_3$ $[M+H]^+$: 463.0652, found: 463.0653.



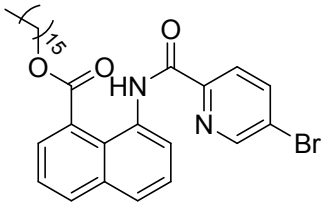
Propyl 8-(picolinamido)-1-naphthoate, **3ab**: yellow solid (30.1 mg, 90%); mp 108-110 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 8.72-8.70 (m, 1H), 8.31-8.28 (m, 1H), 7.99 (dd, J_1 = 8.28 Hz, J_2 = 1.16 Hz, 1H), 7.93-7.89 (m, 2H), 7.86-7.84 (m, 1H), 7.69 (dd, J_1 = 7.08 Hz, J_2 = 1.28 Hz, 1H), 7.62 (t, J = 7.82 Hz, 1H), 7.53-7.46 (m, 2H), 4.11 (t, J = 6.82 Hz, 2H), 1.66-1.57 (m, 2H), 0.83 (t, J = 7.44 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 163.5, 150.0, 149.1, 137.5, 135.1, 131.9, 131.6, 129.1, 128.3, 127.6, 126.8, 126.6, 126.4, 125.9, 124.6, 122.8, 67.6, 21.7, 10.3; HRMS (ESI$^+$): calcd for $C_{20}H_{19}N_2O_3$ $[M+H]^+$: 335.1390, found: 335.1393.



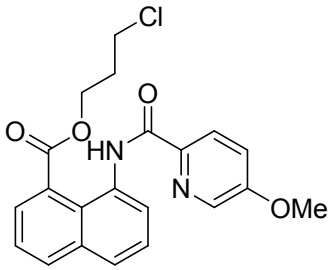
Hexadecyl 8-(picolinamido)-1-naphthoate, **3ac**: yellow solid (17.5 mg, 34%); mp 66-68 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.32 (s, 1H), 8.71-8.70 (m, 1H), 8.30-8.28 (m, 1H), 7.99 (dd, J_1 = 8.28 Hz, J_2 = 1.08 Hz, 1H), 7.93-7.88 (m, 2H), 7.85-7.83 (m, 1H), 7.68 (dd, J_1 = 7.08 Hz, J_2 = 1.24 Hz, 1H), 7.62 (t, J = 7.84 Hz, 1H), 7.52-7.46 (m, 2H), 4.14 (t, J = 6.88 Hz, 2H), 1.60-1.55 (m, 2H), 1.25-1.20 (m, 26H), 0.87 (t, J = 6.68 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 163.5, 150.1, 148.1, 137.5, 135.1, 131.9, 131.7, 129.1, 128.3, 127.5, 126.7, 126.5, 126.4, 125.9, 124.6, 122.9, 66.3, 31.9, 29.7, 29.7, 29.7, 29.6, 29.6, 29.5, 29.4, 29.2, 28.4, 25.9, 22.7, 14.1; HRMS (ESI$^+$): calcd for $C_{33}H_{45}N_2O_3$ $[M+H]^+$: 517.3425, found: 517.3427.



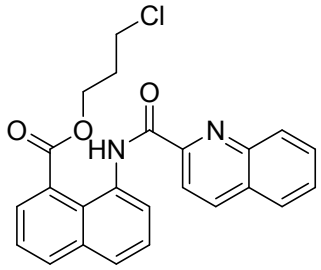
Cyclopentyl 8-(picolinamido)-1-naphthoate, **3ad**: yellow solid (18.7 mg, 52%); mp 95-97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 8.72 (d, J = 4.28 Hz, 1H), 8.29 (d, J = 7.80 Hz, 1H), 7.97 (dd, J_1 = 8.22 Hz, J_2 = 1.04 Hz, 1H), 7.92-7.88 (m, 2H), 7.83 (d, J = 8.08 Hz, 1H), 7.64-7.59 (m, 2H), 7.51-7.45 (m, 2H), 5.25-5.22 (m, 1H), 1.69-1.65 (m, 6H), 1.54-1.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 163.5, 150.1, 148.1, 137.5, 135.1, 131.9, 131.7, 129.4, 128.3, 127.5, 126.7, 126.5, 126.4, 125.8, 124.6, 122.8, 78.8, 32.6, 20.8; HRMS (ESI$^+$): calcd for $C_{22}H_{21}N_2O_3$ $[M+H]^+$: 361.1547, found: 361.1548.



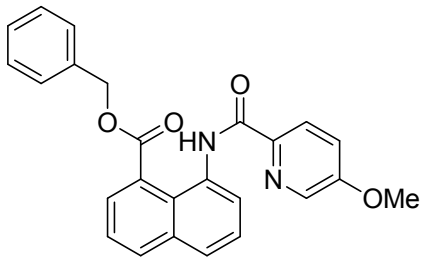
Hexadecyl 8-(5-bromopicolinamido)-1-naphthoate, **3ec**: yellow solid (25.5 mg, 43%); mp 65-68 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.76 (d, J = 1.76 Hz, 1H), 8.20-8.17 (m, 1H), 8.04 (dd, J_1 = 8.32 Hz, J_2 = 2.24 Hz, 1H), 8.00 (dd, J_1 = 8.24 Hz, J_2 = 1.00 Hz, 1H), 7.90-7.84 (m, 2H), 7.71 (dd, J_1 = 7.08 Hz, J_2 = 1.20 Hz, 1H), 7.62 (t, J = 7.84 Hz, 1H), 7.50-7.47 (m, 1H), 4.17 (t, J = 6.26 Hz, 2H), 1.64-1.55 (m, 2H), 1.25-1.22 (m, 26H), 0.88 (t, J = 6.80 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 162.7, 149.3, 148.6, 140.2, 135.1, 132.1, 131.4, 128.9, 128.6, 127.7, 126.8, 126.4, 125.7, 124.6, 124.4, 124.3, 66.3, 31.9, 29.7, 29.7, 29.7, 29.7, 29.6, 29.5, 29.4, 29.3, 28.5, 25.9, 22.7, 14.2; HRMS (ESI$^+$): calcd for $C_{33}H_{44}BrN_2O_3$ $[M+H]^+$: 595.2530, found: 595.2531.



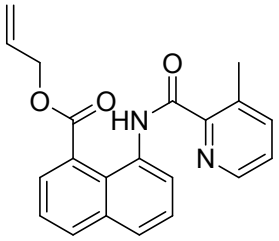
3-Chloropropyl 8-(5-methoxypicolinamido)-1-naphthoate, **3de**: brown solid (20.7 mg, 52%); mp 93-95 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.37 (d, J = 2.68 Hz, 1H), 8.24 (d, J = 8.64 Hz, 1H), 7.99 (dd, J_1 = 8.24 Hz, J_2 = 1.00 Hz, 1H), 7.88-7.82 (m, 2H), 7.67-7.59 (m, 2H), 7.49-7.46 (m, 1H), 7.33 (dd, J_1 = 8.68 Hz, J_2 = 2.84 Hz, 1H), 4.30 (t, J = 6.24 Hz, 2H), 3.93 (s, 3H), 3.51 (t, J = 6.34 Hz, 2H), 2.08-2.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 163.4, 158.3, 142.5, 136.5, 135.0, 132.0, 131.8, 128.7, 128.2, 127.5, 126.9, 126.5, 126.0, 124.6, 124.1, 120.5, 62.8, 55.9, 41.2, 31.3; HRMS (ESI$^+$): calcd for $C_{21}H_{20}ClN_2O_4$ $[M+H]^+$: 399.1106, found: 399.1107.



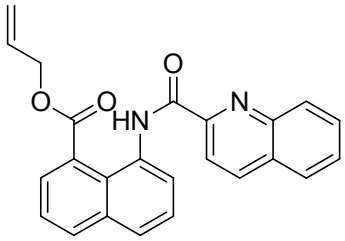
3-Chloropropyl 8-(quinoline-2-carboxamido)-1-naphthoate, **3he**: yellow solid (31.4 mg, 75%); mp 104-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.41-8.36 (m, 2H), 8.32 (d, J = 8.44 Hz, 1H), 8.02 (dd, J_1 = 8.24 Hz, J_2 = 1.04 Hz, 1H), 7.97-7.92 (m, 2H), 7.87-7.82 (m, 2H), 7.70-7.62 (m, 3H), 7.52-7.48 (m, 1H), 4.19 (t, J = 6.22 Hz, 2H), 3.32 (t, J = 6.38 Hz, 2H), 1.90-1.83 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 163.6, 149.6, 146.4, 137.8, 135.1, 132.1, 131.8, 130.5, 129.8, 129.5, 128.7, 128.3, 128.3, 127.9, 127.6, 126.7, 126.6, 125.9, 124.6, 119.1, 62.6, 40.9, 31.2; HRMS (ESI$^+$): calcd for $C_{24}H_{20}ClN_2O_3$ $[M+H]^+$: 419.1157, found: 419.1159.



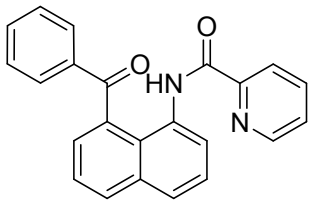
Benzyl 8-(5-methoxypicolinamido)-1-naphthoate, **3df**: brown oil (8.7 mg, 21%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.17 (s, 1H), 8.31 (d, J = 2.76 Hz, 1H), 8.23 (d, J = 8.64 Hz, 1H), 7.98 (dd, J_1 = 8.26 Hz, J_2 = 1.10 Hz, 1H), 7.89 (d, J = 7.44 Hz, 1H), 7.83 (d, J = 8.16 Hz, 1H), 7.67-7.59 (m, 2H), 7.47-7.43 (m, 1H), 7.32-7.28 (m, 6H), 5.22 (s, 2H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 163.4, 158.2, 142.6, 136.4, 135.5, 135.0, 132.0, 131.8, 128.7, 128.5, 128.3 128.3, 128.0, 127.4, 126.8, 126.5, 126.0, 124.6, 124.2, 120.4, 67.6, 55.8; HRMS (ESI$^+$): calcd for $C_{25}H_{21}N_2O_4$ $[M+H]^+$: 413.1496, found: 413.1499.



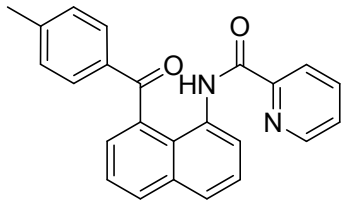
Allyl 8-(3-methylpicolinamido)-1-naphthoate, **3bg**: brown solid (8.0 mg, 23%); mp 119-121 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.35 (s, 1H), 8.55-8.53 (m, 1H), 7.99 (dd, J_1 = 8.24 Hz, J_2 = 1.12 Hz, 1H), 7.87-7.83 (m, 2H), 7.68-7.60 (m, 3H), 7.50-7.46 (m, 1H), 7.42-7.38 (m, 1H), 5.89-5.79 (m, 1H), 5.23-5.12 (m, 2H), 4.57 (dt, J_1 = 5.77 Hz, J_2 = 1.26 Hz, 2H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 165.0, 147.0, 145.4, 141.1, 136.4, 135.1, 131.9, 131.8, 131.6, 128.9, 128.2, 127.4, 126.9, 126.4, 126.2, 126.1, 124.6, 118.6, 66.4, 20.8; HRMS (ESI$^+$): calcd for $C_{21}H_{19}N_2O_3$ $[M+H]^+$: 347.1390, found: 347.1392.



Allyl 8-(quinoline-2-carboxamido)-1-naphthoate, **3hg**: brown solid (12.2 mg, 32%); mp 109-111 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (s, 1H), 8.41-8.35 (m, 2H), 8.31 (d, J = 8.48 Hz, 1H), 8.02-7.92 (m, 3H), 7.87-7.81 (m, 2H), 7.73-7.62 (m, 3H), 7.52-7.48 (m, 1H), 5.78-5.67 (m, 1H), 5.05-4.95 (m, 2H), 4.55 (dt, J_1 = 5.76 Hz, J_2 = 1.36 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 163.6, 149.7, 146.4, 137.7, 135.1, 132.0, 131.8, 131.5, 130.4, 129.9, 129.5, 128.8, 128.4, 128.2, 127.8, 127.5, 126.6, 126.5, 125.9, 124.7, 119.2, 118.4, 66.4; HRMS (ESI$^+$): calcd for $C_{24}H_{19}N_2O_3$ $[M+H]^+$: 383.1390, found: 383.1392.

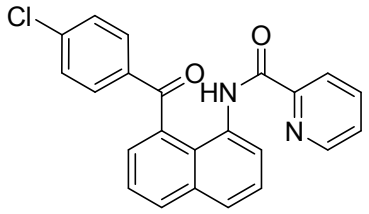


N-(8-benzoylnaphthalen-1-yl)picolinamide, **3ah:** White solid (12.7 mg, 36%); mp 144-146 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.72 (s, 1H), 8.54-8.52 (m, 1H), 8.04-8.02 (m, 1H), 7.92 (d, J = 7.92 Hz, 1H), 7.80-7.78 (m, 1H), 7.74-7.68 (m, 2H), 7.64-7.60 (m, 1H), 7.56-7.52 (m, 1H), 7.50-7.48 (m, 2H), 7.42-7.32 (m, 3H), 7.14-7.10 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 163.1, 149.2, 147.9, 137.0, 136.9, 136.0, 135.1, 133.2, 131.7, 130.5, 130.0, 128.0, 127.9, 127.8, 126.9, 126.6, 126.5, 126.2, 124.9, 122.1; HRMS (ESI$^+$): calcd for $C_{23}H_{16}N_2O_2$ $[M+H]^+$: 353.1285, Found: 353.1287.

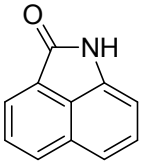


N-(8-(4-methylbenzoyl)naphthalen-1-yl)picolinamide, **3ai:** White solid (13.9 mg, 38%); mp 166-

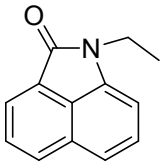
168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.72 (s, 1H), 8.55-8.53 (m, 1H), 8.03-8.00 (m, 1H), 7.91 (d, J = 8.20 Hz, 1H), 7.81-7.79 (m, 1H), 7.75-7.68 (m, 2H), 7.63-7.59 (m, 1H), 7.55-7.52 (m, 1H), 7.42-7.38 (m, 4H), 6.91 (d, J = 7.96 Hz, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.2, 163.2, 149.3, 147.9, 144.1, 136.8, 136.2, 135.1, 134.6, 131.8, 130.4, 130.2, 128.6, 127.9, 127.7, 126.8, 126.5, 126.4, 126.2, 124.9, 122.1, 21.6; HRMS (ESI$^+$): calcd for $C_{24}H_{18}N_2O_2$ $[M+H]^+$: 367.1441, Found: 367.1442.



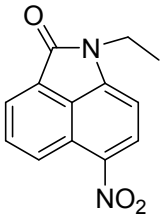
N-(8-(4-chlorobenzoyl)naphthalen-1-yl)picolinamide, **3aj:** White solid (11.8 mg, 36%); mp 174-177 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.54 (d, J = 4.72 Hz, 1H), 8.03 (d, J = 8.12 Hz, 1H), 7.92 (d, J = 8.04 Hz, 1H), 7.82-7. 81 (m, 1H), 7.77-7.73 (m, 1H), 7.71-7.69 (m, 1H), 7.64-7.61 (m, 1H), 7.56-7.53 (m, 1H), 7.44-7.37 (m, 4H), 7.07 (d, J = 8.56 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 163.2, 149.1, 147.9, 139.7, 137.1, 135.4, 135.3, 135.1, 131.6, 131.3, 130.7, 128.2, 128.2, 128.0, 127.2, 126.7, 126.4, 126.4, 124.9, 122.2; HRMS (ESI$^+$): calcd for $C_{23}H_{15}ClN_2O_2$ $[M+H]^+$: 387.0895, Found: 387.0894.



Benzo[cd]indol-2(1H)-one, **4a**: yellow solid (18.6 mg, 55%); mp 173-176 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.11 (d, J = 7.00 Hz, 1H), 8.05 (d, J = 8.08 Hz, 1H), 7.76-7.72 (m, 1H), 7.56 (d, J = 8.44 Hz, 1H), 7.48-7.44 (m, 1H), 7.03 (d, J = 7.00 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 137.2, 131.2, 129.4, 128.7, 126.8, 126.3, 124.5, 120.4, 106.7; HRMS (ESI$^+$): calcd for $C_{11}H_8NO$ $[M+H]^+$: 170.0600, found: 170.0599.

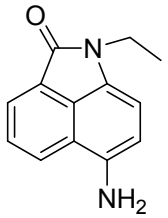


1-Ethylbenzo[cd]indol-2(1H)-one, **5a**: yellow solid (189 mg, 96%); mp 65-68 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 6.96 Hz, 1H), 7.91 (d, J = 8.12 Hz, 1H), 7.64-7.60 (m, 1H), 7.45-7.37 (m, 2H), 6.83 (d, J = 6.88 Hz, 1H), 3.92 (q, J = 7.24 Hz, 2H), 1.34 (t, J = 7.24 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 139.0, 130.6, 129.0, 128.5, 128.4, 126.7, 125.1, 124.0, 120.1, 104.8, 34.9, 14.1; HRMS (ESI$^+$): calcd for $C_{13}H_{12}NO$ $[M+H]^+$: 198.0913, found: 198.0915.

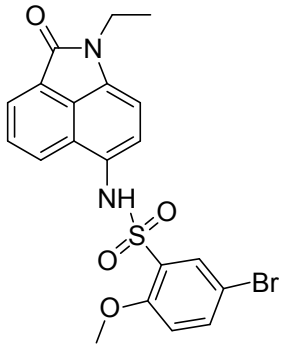


1-Ethyl-6-nitrobenzo[cd]indol-2(1H)-one, **6a**: yellow solid (155 mg, 67%); mp 158-161 °C; ^{1}H

NMR (400 MHz, $CDCl_3$) δ 8.89 (d, J = 8.52 Hz, 1H), 8.56 (d, J = 8.00 Hz, 1H), 8.06 (d, J = 6.96 Hz, 1H), 7.86 (t, J = 7.76 Hz, 1H), 6.92 (d, J = 8.00 Hz, 1H), 3.99 (q, J = 7.20 Hz, 2H), 1.40 (t, J = 7.20 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 145.6, 138.9, 131.9, 129.9,129.9, 126.0, 125.6, 125.3, 122.5, 102.9, 35.2, 13.9; HRMS (ESI^+): calcd for $C_{13}H_{11}N_2O_3$ $[M+H]^+$: 243.0764, found: 243.0762.



1-Ethyl-6-nitrobenzo[cd]indol-2(1H)-one, **7a**: red solid (105 mg, 77%); mp 181-183 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 7.00 Hz, 1H), 8.00 (d, J = 8.16 Hz, 1H), 7.69-7.65 (m, 1H), 6.73 (d, J = 7.44 Hz, 1H), 6.64 (d, J = 7.44 Hz, 1H), 3.94 (q, J = 7.24 Hz, 2H), 3.41 (s, 2H), 1.35 (t, J = 7.24 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 138.4, 131.1, 127.6, 127.4, 125.6, 125.3, 124.3, 121.5, 109.7, 106.5, 34.9, 14.1; HRMS (ESI^+): calcd for $C_{13}H_{13}N_2O$ $[M+H]^+$: 213.1022, found: 213.1023.



5-bromo-N-(1-ethyl-2-oxo-1,2-dihydrobenzo[cd]indol-6-yl)-2-methoxybenzenesulfonamide, **8a**: yellow solid (202 mg, 88%); mp 209-211 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 8.28 Hz, 1H), 8.00 (d, J = 6.96 Hz, 1H), 7.80-7.79 (m, 2H), 7.69-7.65 (m, 1H), 7.53 (dd, J_1 = 8.80 Hz, J_2 = 2.48 Hz, 1H), 7.17 (d, J = 7.56 Hz, 1H), 6.90 (d, J = 8.88 Hz, 1H), 6.71 (d, J = 7.60 Hz, 1H), 4.06 (s, 3H), 3.88 (q, J = 7.20 Hz, 2H), 1.30 (t, J = 7.20 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 155.4, 138.1, 137.6, 133.2, 129.0, 128.2, 127.0, 126.8, 126.4, 126.1, 125.5, 124.8, 124.4, 113.9, 112.8, 104.8, 56.7, 35.0, 14.0; HRMS (ESI^+): calcd for $C_{20}H_{18}BrN_2O_4S$ $[M+H]^+$: 461.0165 , found: 461.0167.

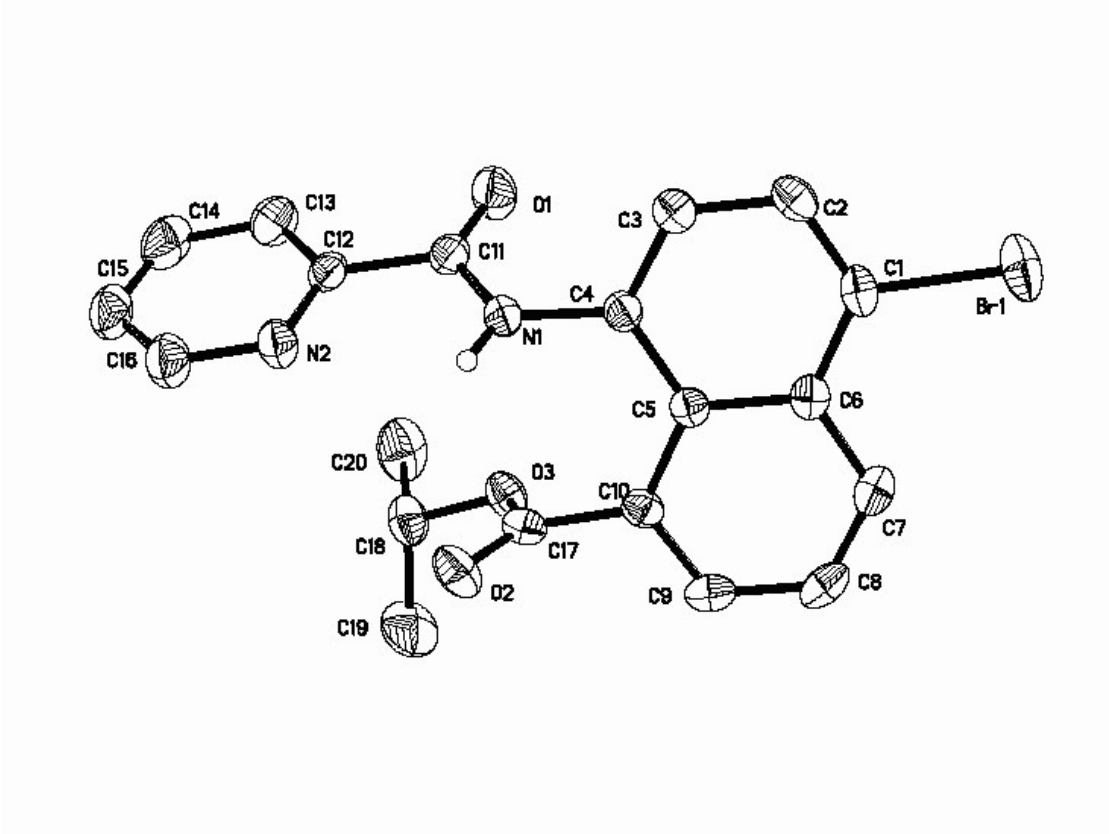
5. References

[1]. R. Shang, L. Ilies, E. Nakamura, *J. Am. Chem. Soc*. **2015**, *137*, 7660.

[2]. (a) X. Xue, Y. Zhang, Z. Liu, M. Song, Y. Xing, Q. Xiang, Z. Wang, Z. Tu, Y. Zhou, K. Deng, Y. Xu, *J. Med. Chem.* **2016**, *59*, 1565; (b) Y. Feng, S. Xiao, Y. Chen, H. Jiang, N. Liu, C. Luo, S. Chen, H. Chen, *Eur. J. Med. Chem.* **2018**, *152*, 264.

6. The Single Crystal X-ray Diffraction Study

The Single Crystal X-ray Diffraction Study of **3na**



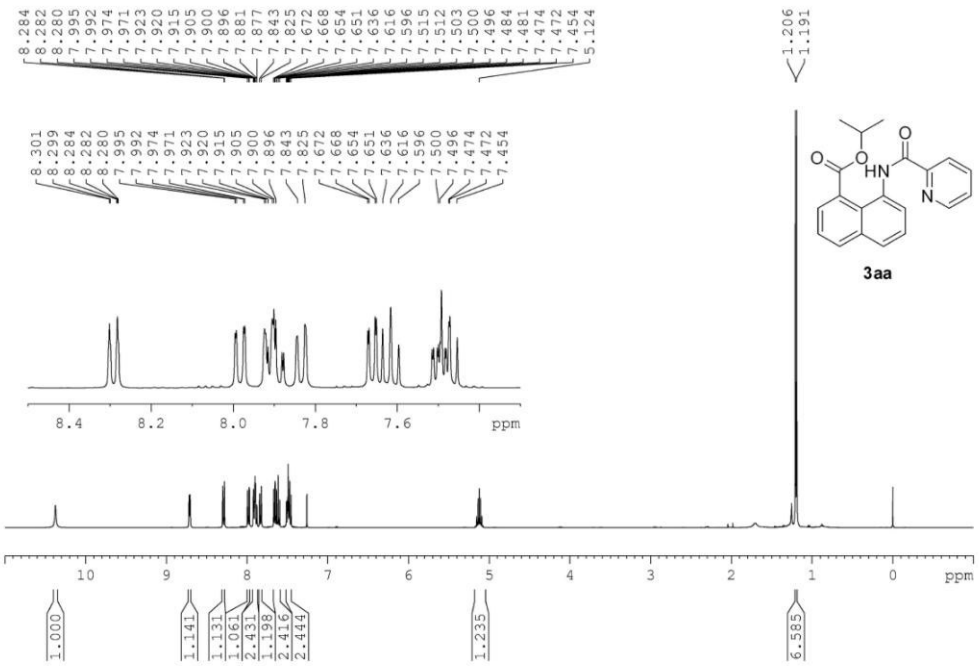
CCDC 1956109 (**3na**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www. ccdc.cam.ac.uk/data_request/cif.

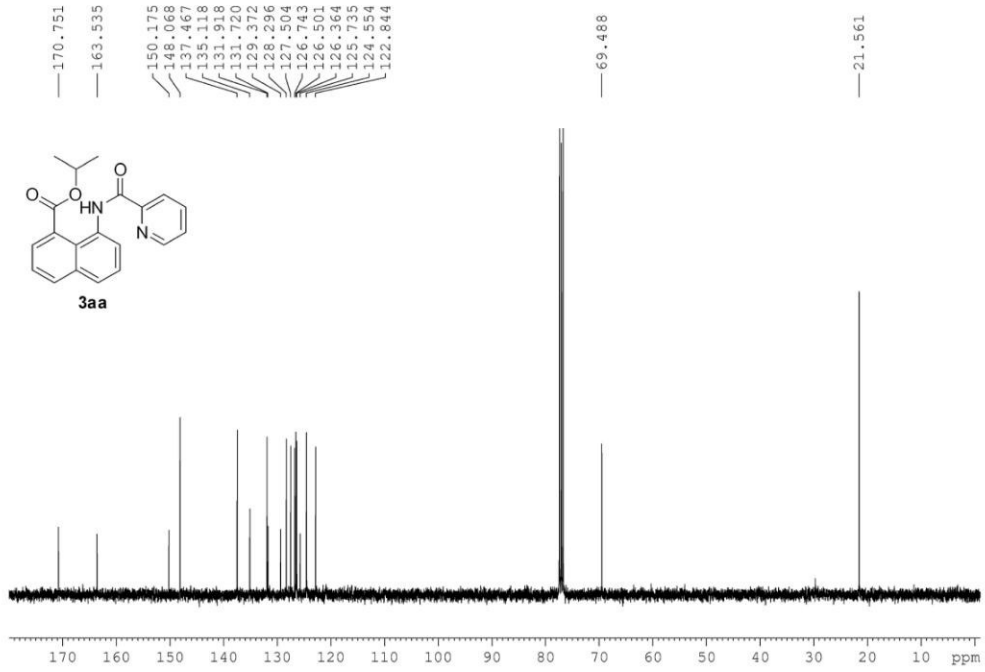
Table S3 Crystal data and structure refinement for CCDC 1956109.

Empirical formula	$C_{20}H_{17}BrN_2O_3$
Formula weight	413.26
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.6385(13)
b/Å	14.3268(8)
c/Å	7.7041(5)
α/°	90
β/°	100.731(7)
γ/°	90
Volume/Å^3	1804.3(2)
Z	4
ρ_{calc}g/cm^3	1.521
μ/mm^{-1}	3.296
F(000)	840.0

Crystal size/mm^3	0.19 × 0.14 × 0.11
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.206 to 134.16
Index ranges	-19 ≤ h ≤ 13, -17 ≤ k ≤ 16, -8 ≤ l ≤ 9
Reflections collected	6920
Independent reflections	3221 [R_{int} = 0.0468, R_{sigma} = 0.0652]
Data/restraints/parameters	3221/0/242
Goodness-of-fit on F^2	1.053
Final R indexes [I>=2σ (I)]	R_1 = 0.0486, wR_2 = 0.1062
Final R indexes [all data]	R_1 = 0.0755, wR_2 = 0.1265
Largest diff. peak/hole / e Å^{-3}	0.35/-0.43

7. Copies of ^{1}H, ^{13}C NMR Spectra for the Products

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21.561
3aa
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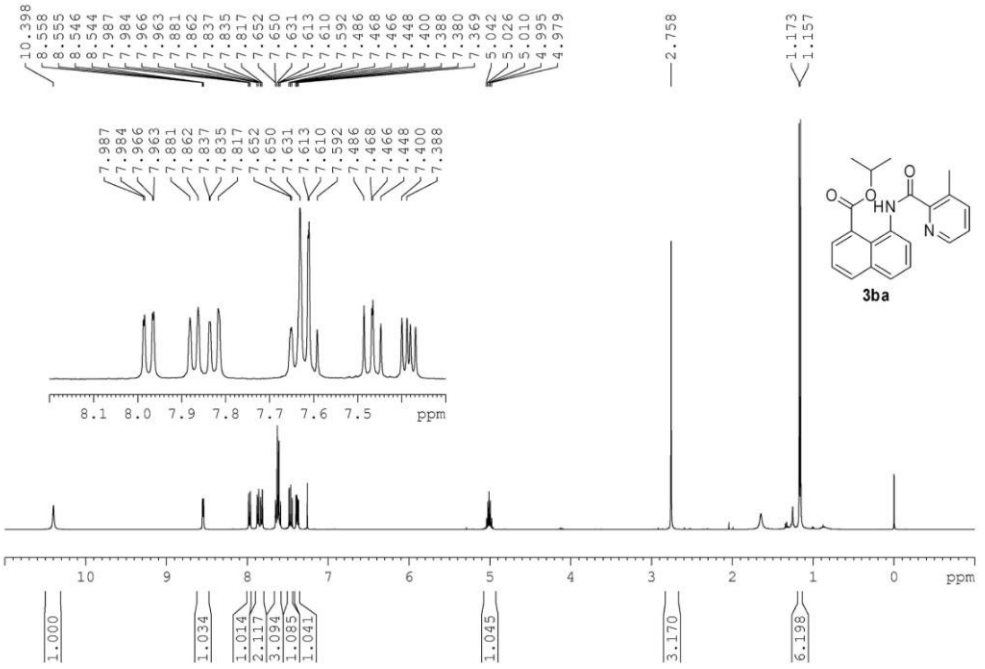
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7.817
7.652
7.650
7.631
7.613
7.610
7.592
7.486
7.468
7.466
7.448
7.400
7.388
7.380
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5.026
5.010
4.995
4.979
2.758
1.173
1.157
3ba
8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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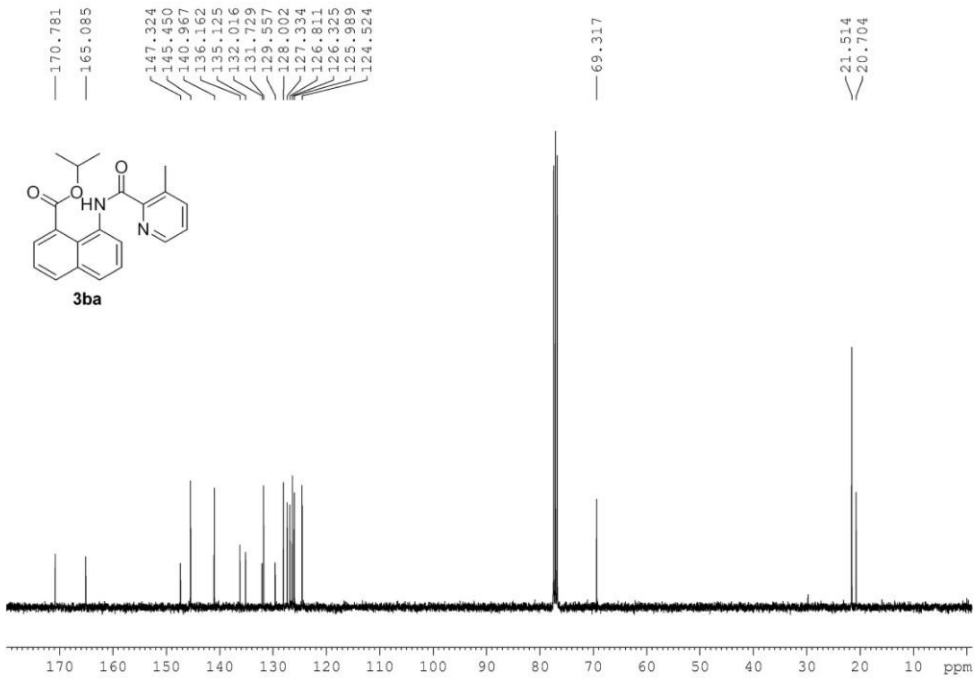
3.094
1.085
1.041
1.045
3.170
6.198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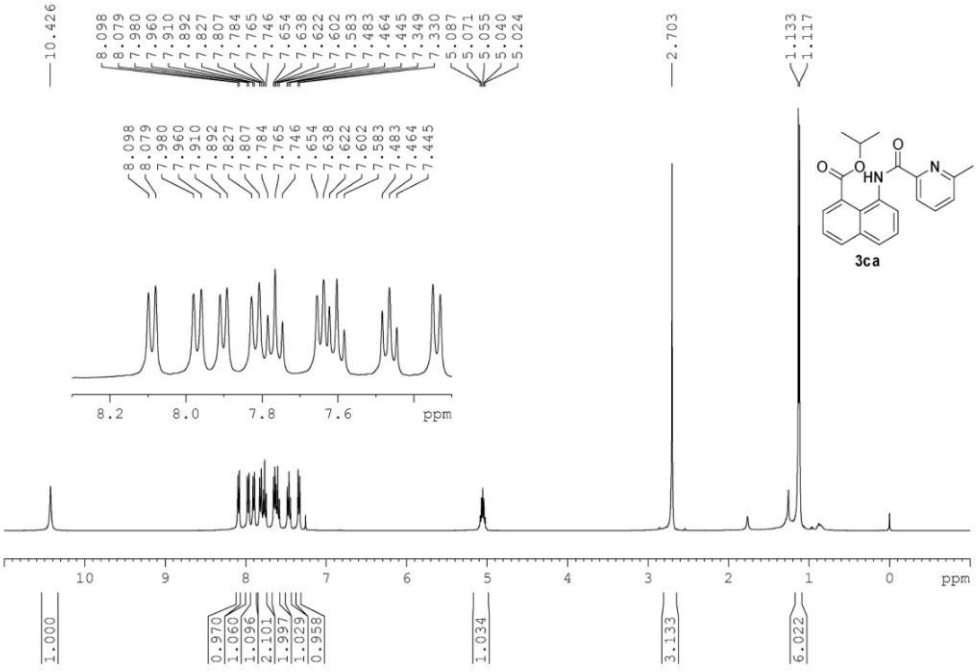
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5.071
5.055
5.040
5.024
2.703
1.133
1.117
3ca
8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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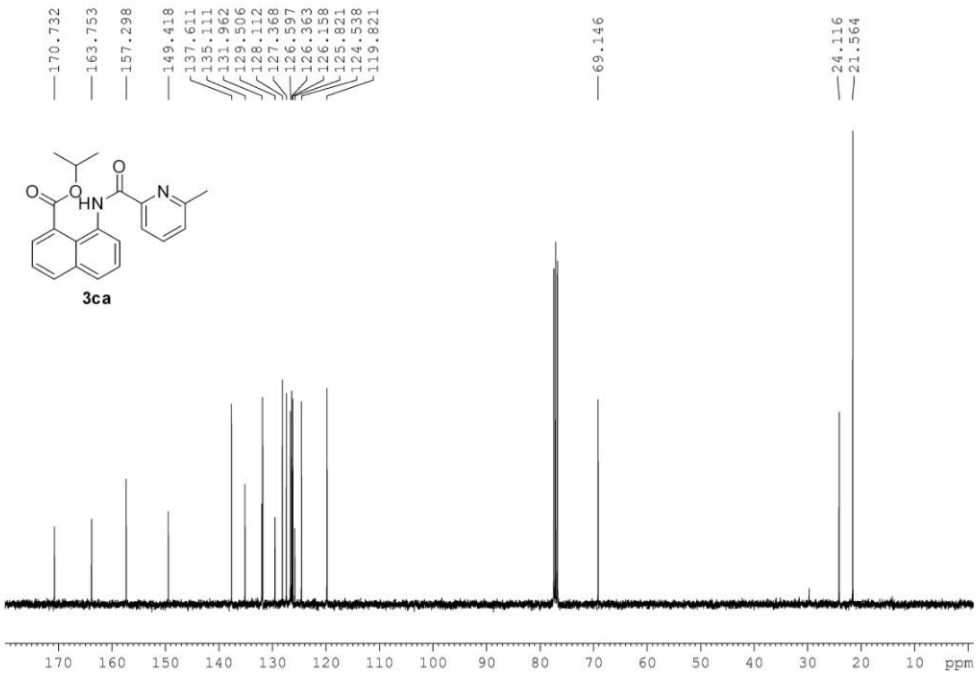
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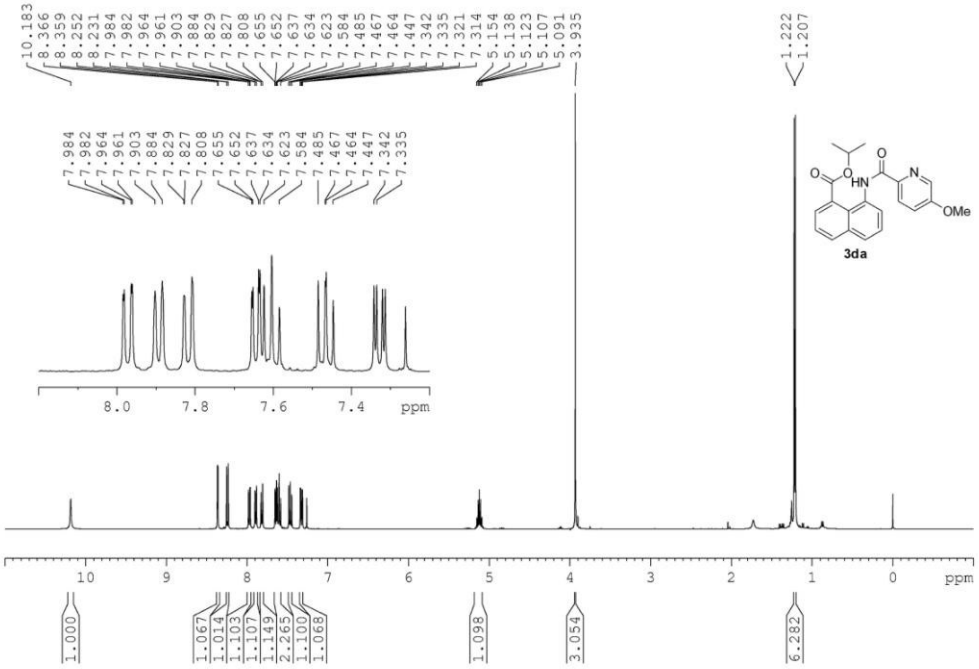
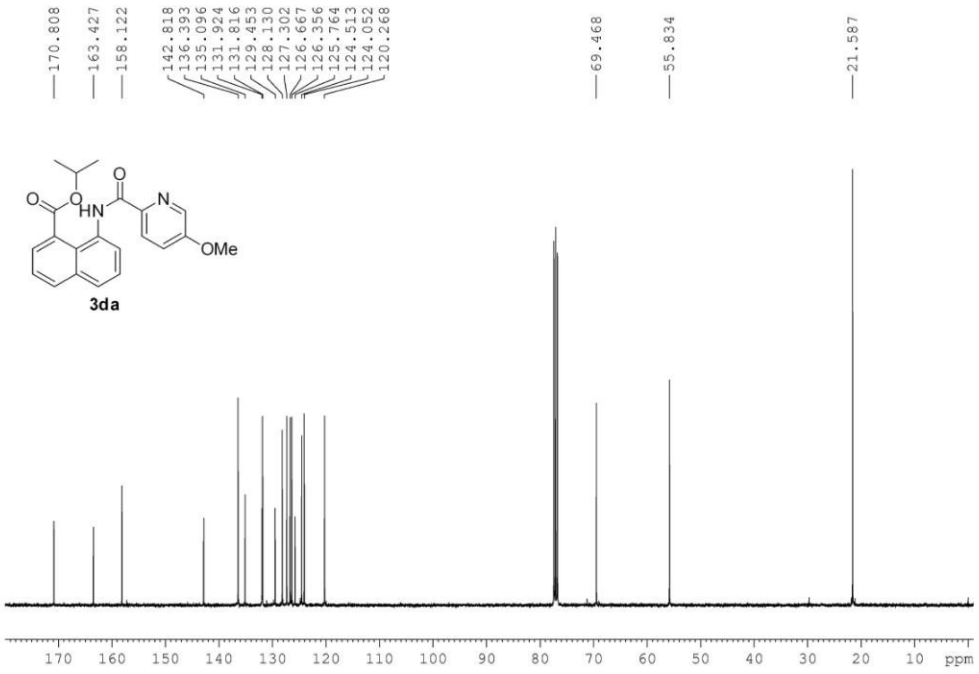
125.821
124.538
119.821
69.146
24.116
21.564
3ca
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.183
8.366
8.359
8.252
8.231
7.984
7.982
7.964
7.961
7.903
7.884
7.829
7.827
7.808
7.655
7.652
7.637
7.634
7.623
7.584
7.485
7.467
7.464
7.447
7.342
7.335
7.321
7.314
5.154
5.138
5.123
5.107
5.091
3.935
1.222
1.207
3da
8.0 7.8 7.6 7.4 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.067
1.014
1.103
1.107
1.149
2.265
1.100
1.068
1.098
3.054
6.282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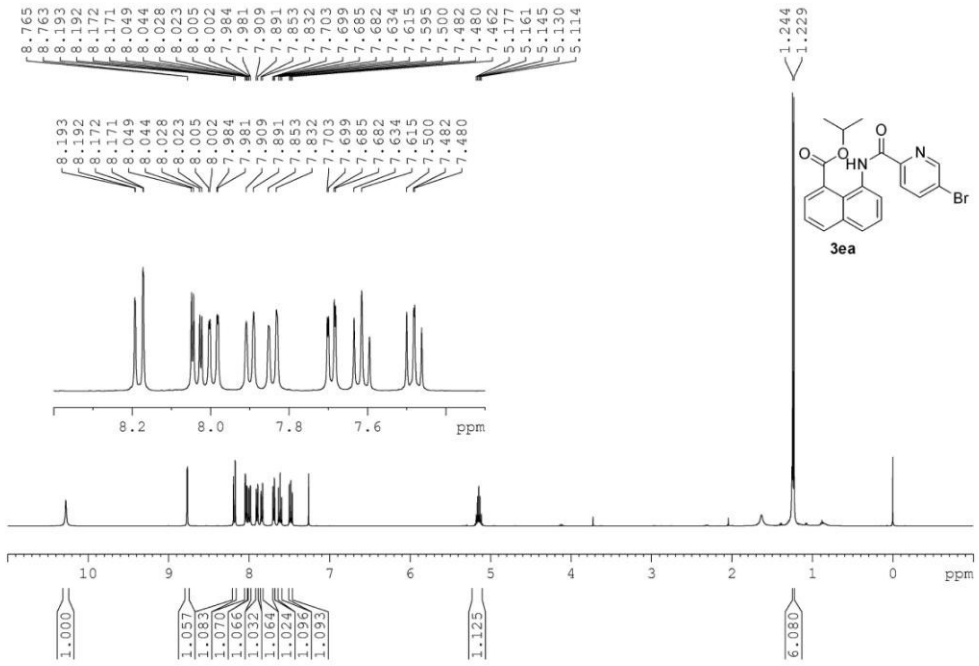
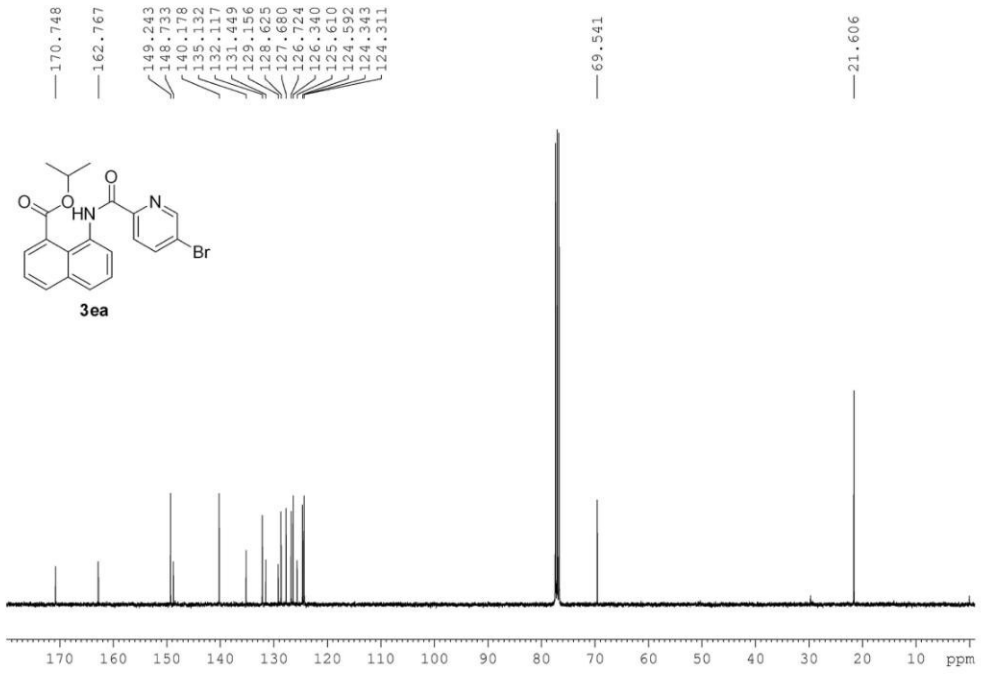
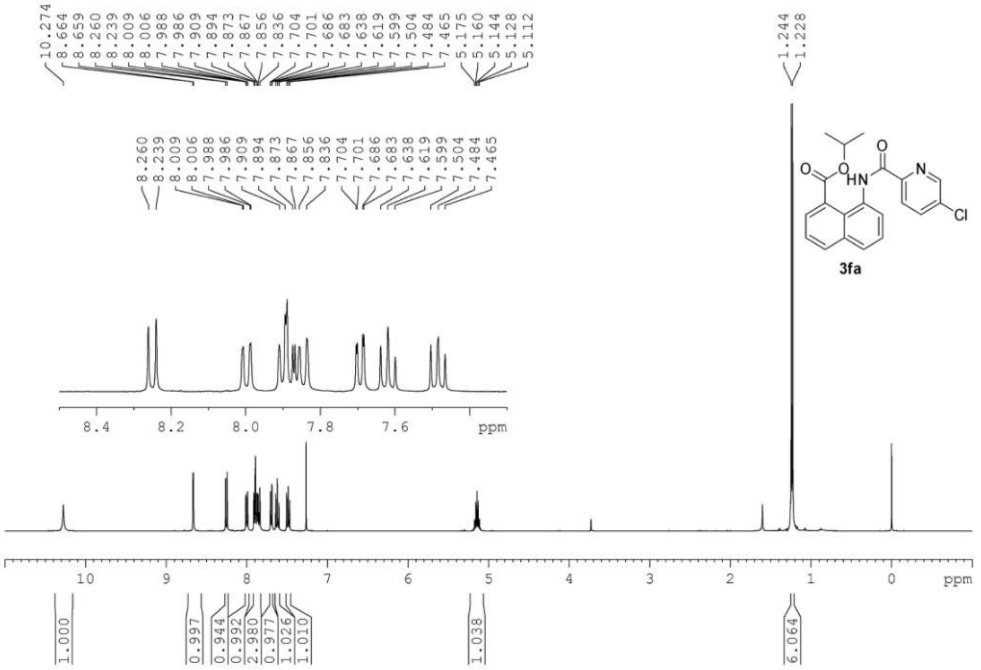
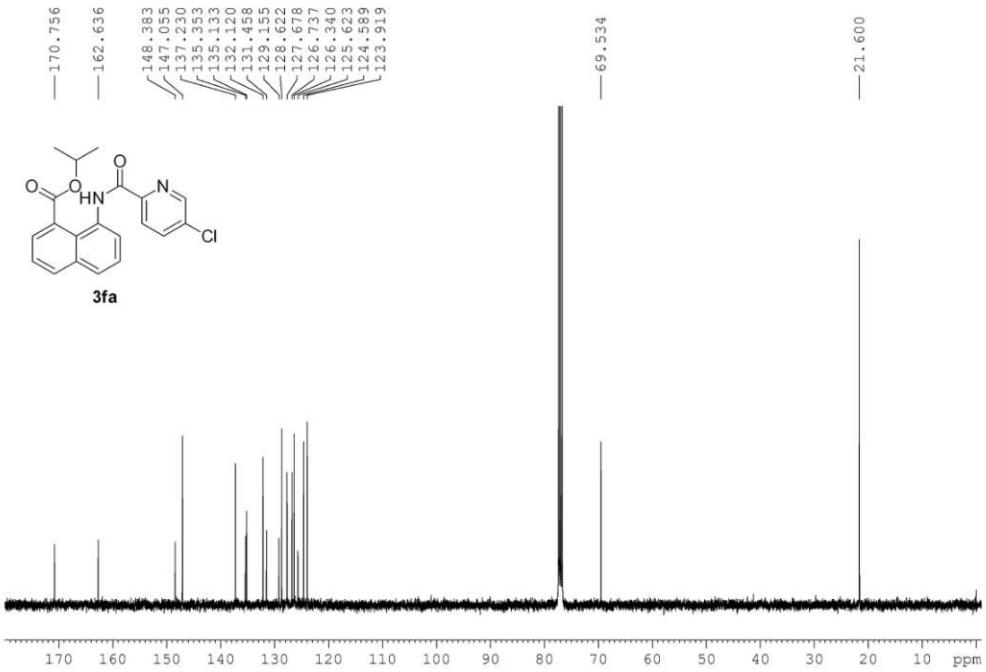
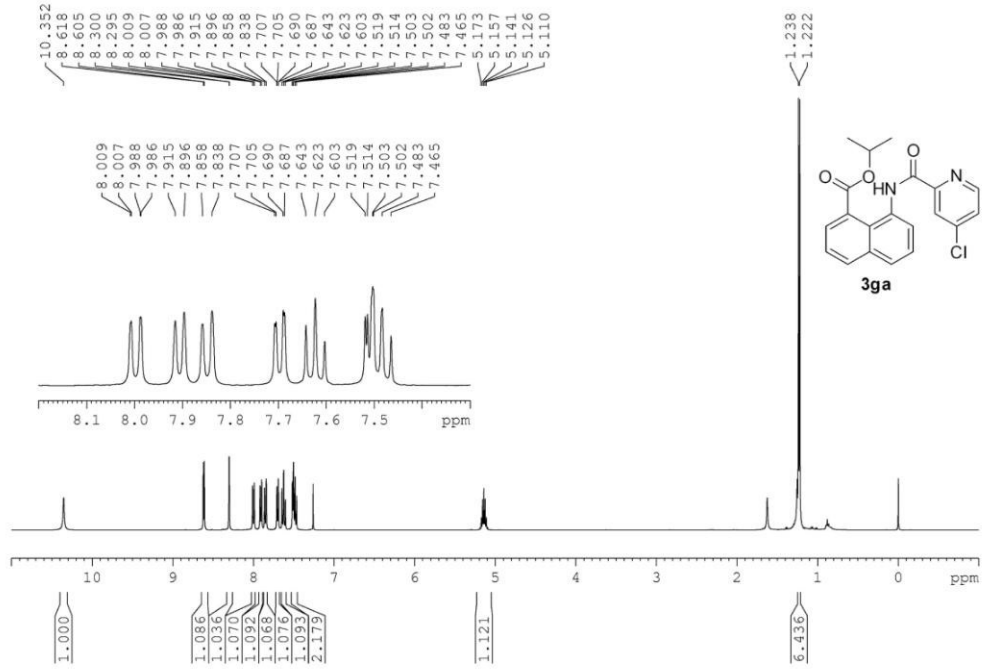
163.427
158.122
142.818
136.393
135.096
131.924
131.816
129.453
128.130
127.302
126.667
126.356
125.764
124.513
124.052
120.268
69.468
55.834
21.587
OMe
3da
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

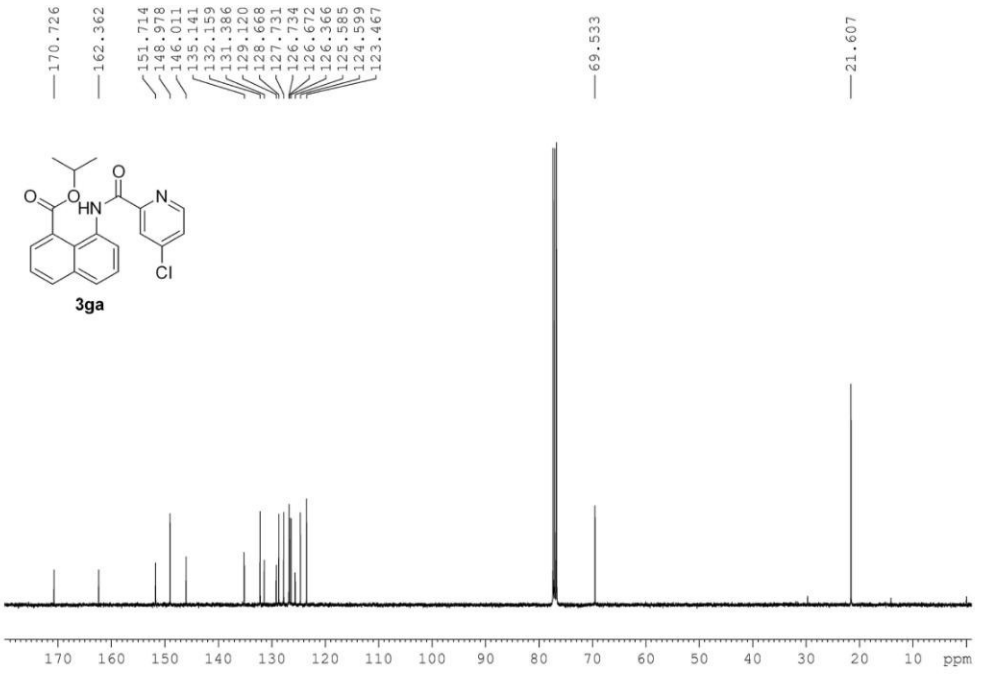

8.765
8.763
8.193
8.192
8.172
8.171
8.049
8.044
8.028
8.023
8.005
8.002
7.984
7.981
7.909
7.891
7.853
7.832
7.703
7.699
7.685
7.682
7.634
7.615
7.595
7.500
7.482
7.480
7.462
5.177
5.161
5.145
5.130
5.114
1.244
1.229
Br
3ea
8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.057
1.083
1.070
1.066
1.032
1.064
1.024
1.096
1.093
1.125
6.080

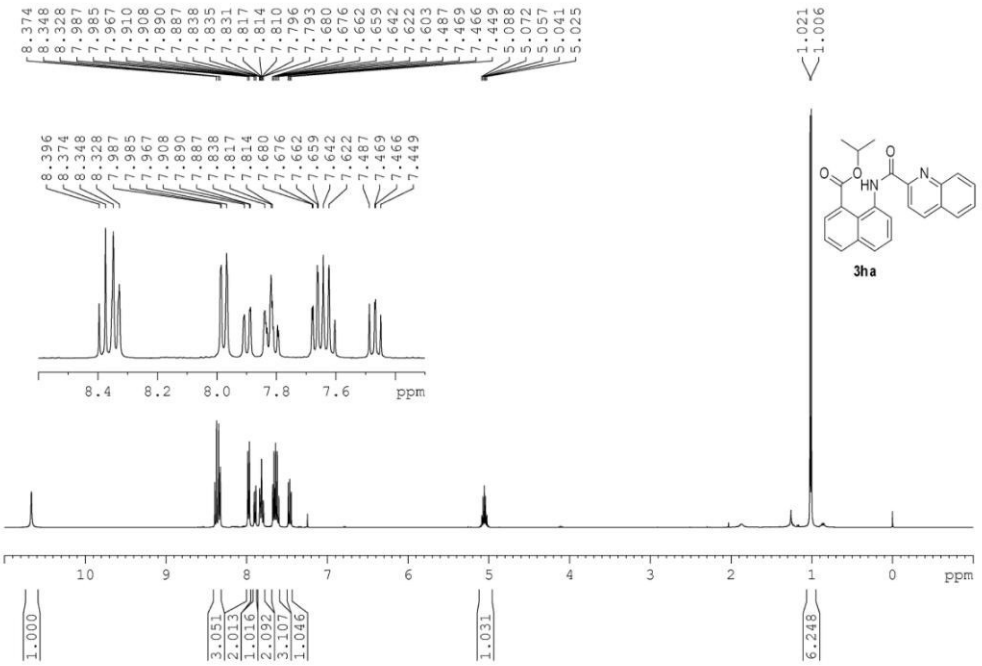

170.748
162.767
149.243
148.733
140.178
135.132
132.117
131.449
129.156
128.625
127.680
126.724
126.340
125.610
124.592
124.343
124.311
69.541
21.606
O
O
HN
O
N
Br
3ea
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

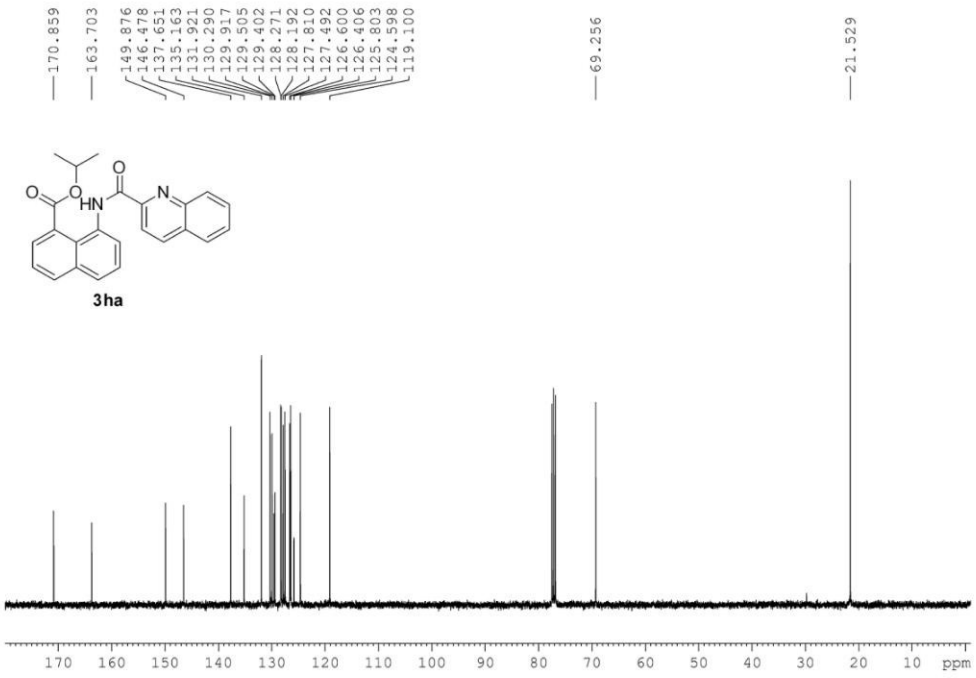

10.274
8.664
8.659
8.260
8.239
8.009
8.006
7.988
7.986
7.909
7.894
7.873
7.867
7.856
7.836
7.704
7.701
7.686
7.683
7.638
7.619
7.599
7.504
7.484
7.465
5.175
5.160
5.144
5.128
5.112
1.244
1.228
O
O
HN
O
N
Cl
3fa
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.997
0.944
0.992
2.980
0.977
1.026
1.010
1.038
6.064

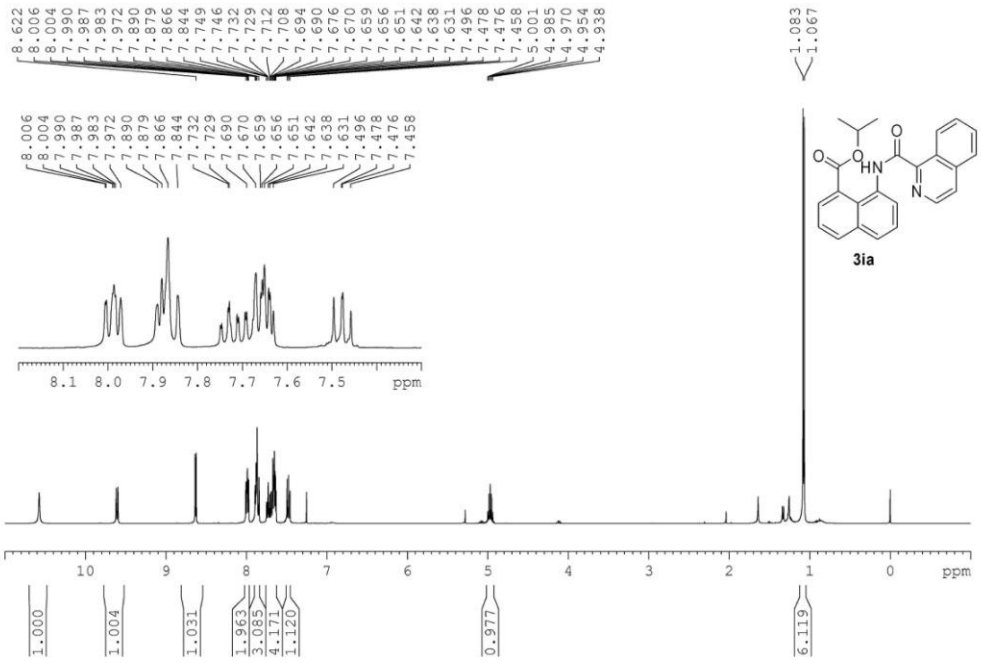

170.756
162.636
148.383
147.055
137.230
135.353
135.133
132.120
131.458
129.155
128.622
127.678
126.737
126.340
125.623
124.589
123.919
69.534
21.600
3fa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

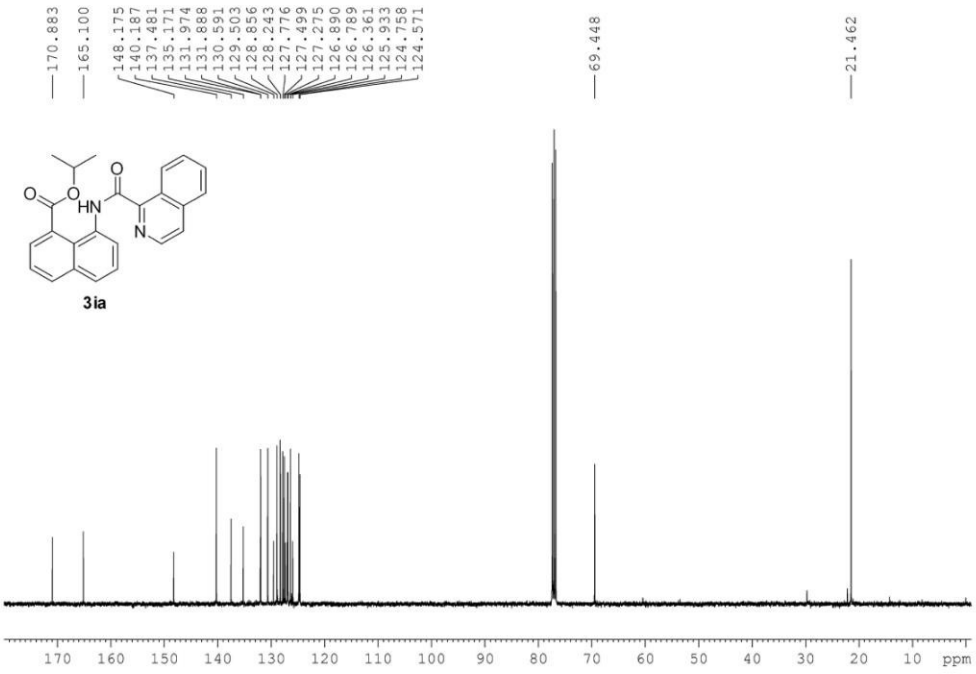

10.352
8.618
8.605
8.300
8.295
8.009
8.007
7.988
7.986
7.915
7.896
7.858
7.838
7.707
7.705
7.690
7.687
7.643
7.623
7.603
7.519
7.514
7.503
7.502
7.483
7.465
5.173
5.157
5.141
5.126
5.110
1.238
1.222
3ga
8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.086
1.036
1.070
1.092
1.068
1.076
1.093
2.179
1.121
6.436

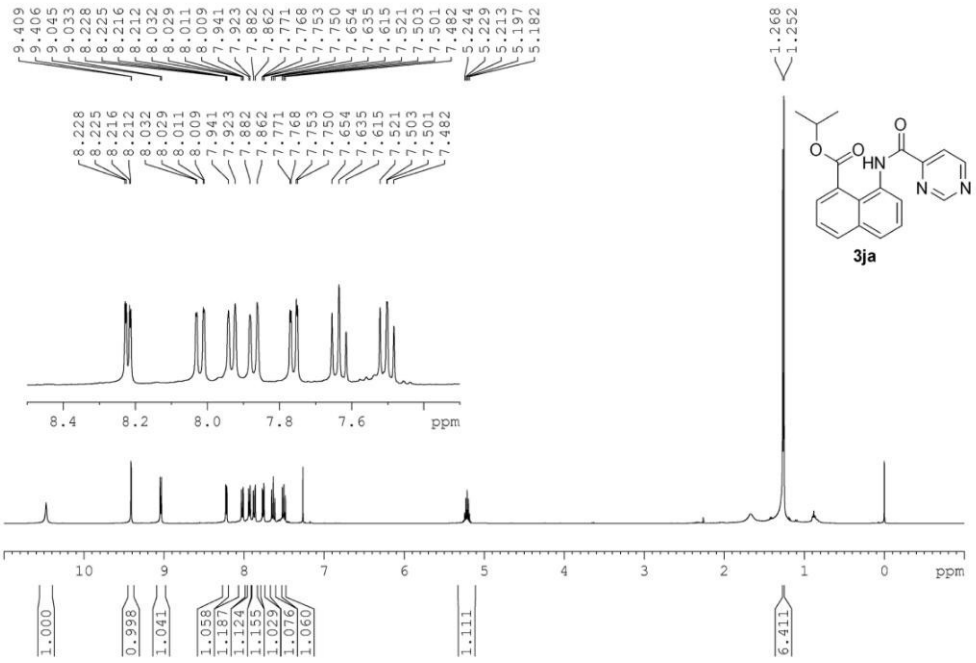

170.726
162.362
151.714
148.978
146.011
135.141
132.159
131.386
129.120
128.668
127.731
126.734
126.672
126.366
125.585
124.599
123.467
69.533
21.607
3ga
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

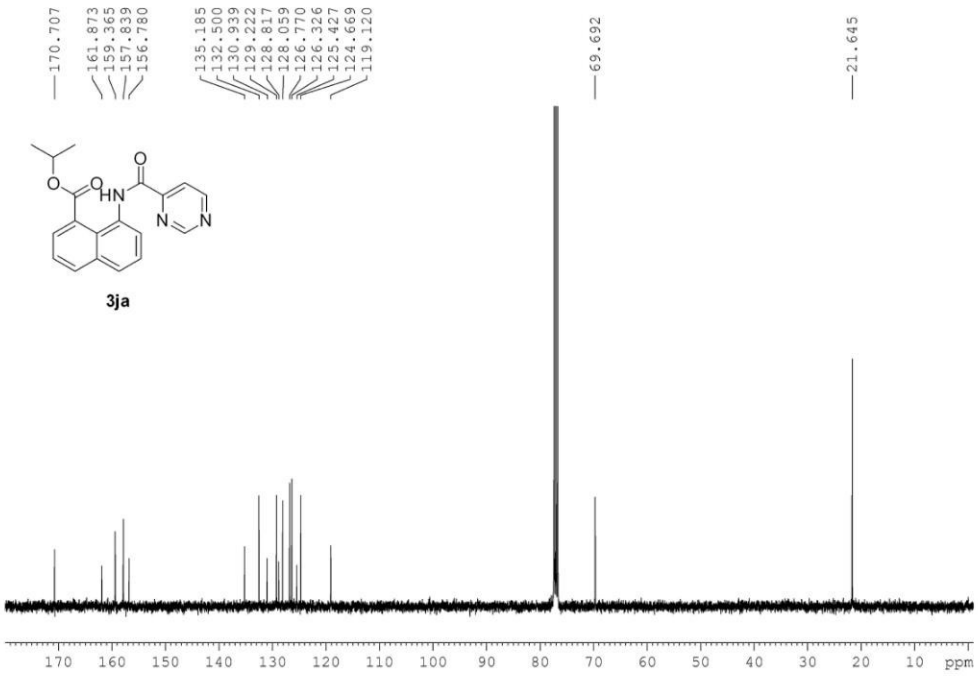

8.374
8.348
8.328
7.987
7.985
7.967
7.910
7.908
7.890
7.887
7.838
7.835
7.831
7.817
7.814
7.810
7.796
7.793
7.680
7.676
7.662
7.659
7.642
7.622
7.603
7.487
7.469
7.466
7.449
5.088
5.072
5.057
5.041
5.025
1.021
1.006
3ha
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
3.051
2.013
1.016
2.092
3.107
1.046
1.031
6.248

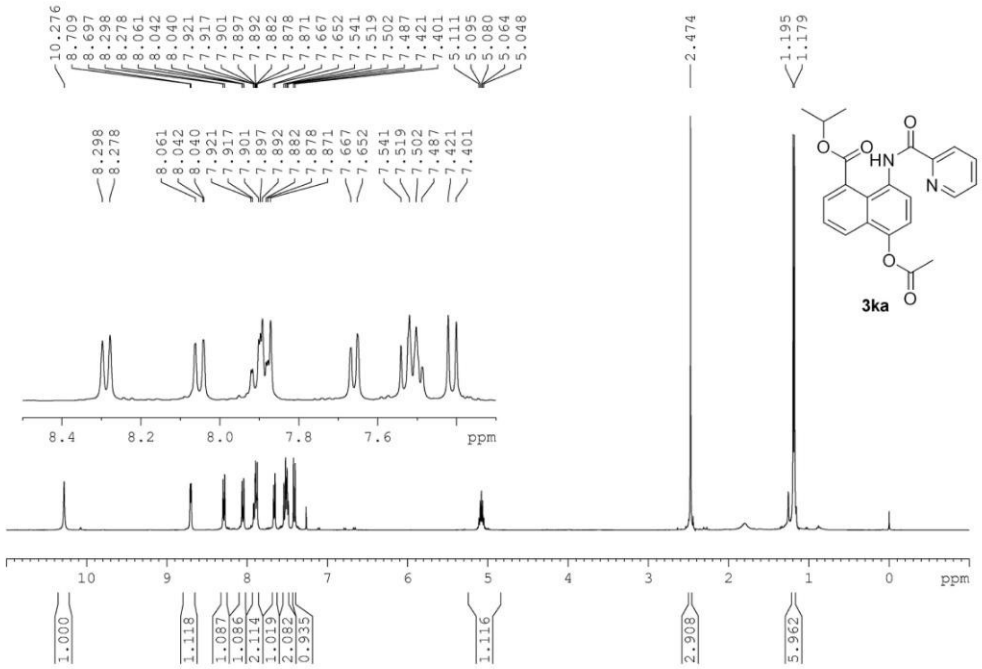

170.859
163.703
149.876
146.478
137.651
135.163
131.921
130.290
129.917
129.505
129.402
128.271
128.192
127.810
127.492
126.600
126.406
125.803
124.598
119.100
69.256
21.529
3ha
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

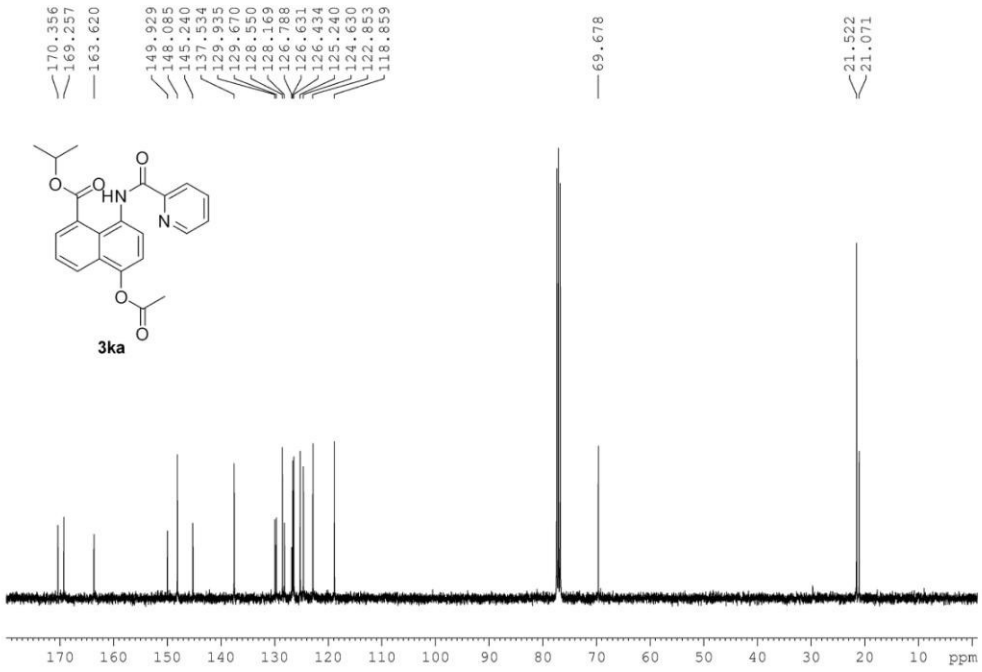

8.622
8.006
8.004
7.990
7.987
7.983
7.972
7.890
7.879
7.866
7.844
7.749
7.746
7.732
7.729
7.712
7.708
7.694
7.690
7.676
7.670
7.659
7.656
7.651
7.642
7.638
7.631
7.496
7.478
7.476
7.458
5.001
4.985
4.970
4.954
4.938
1.083
1.067
3ia
8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.004
1.031
1.963
3.085
4.171
1.120
0.977
6.119

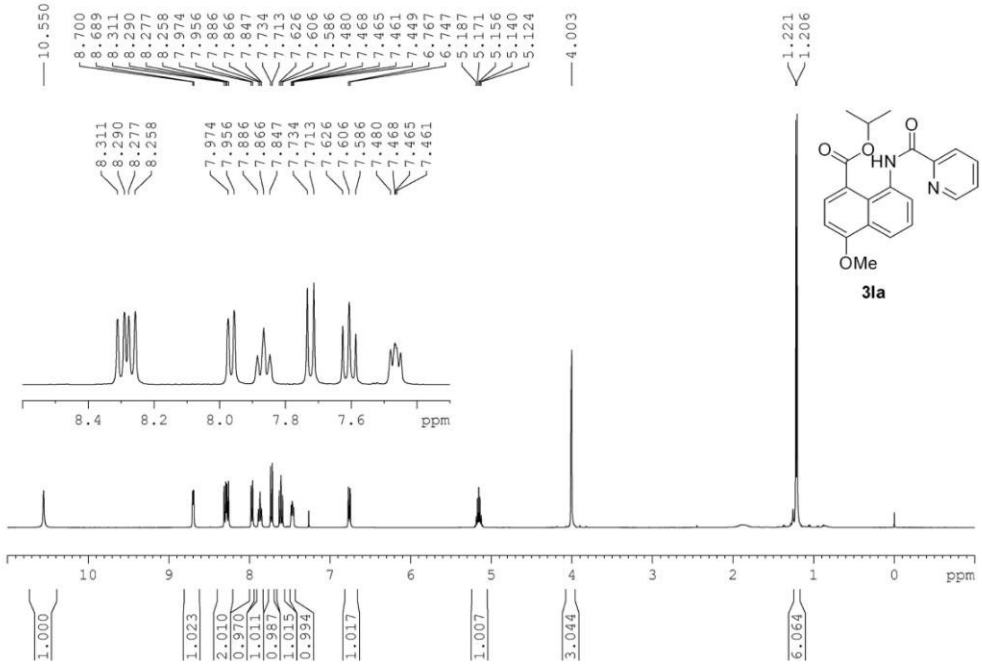

170.883
165.100
148.175
140.187
137.481
135.171
131.974
131.888
130.591
129.503
128.856
128.443
127.776
127.499
127.275
126.890
126.789
126.361
125.933
124.758
124.571
69.448
21.462
3ia
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


9.409
9.406
9.045
9.033
8.228
8.225
8.216
8.212
8.032
8.029
8.011
8.009
7.941
7.923
7.882
7.862
7.771
7.768
7.753
7.750
7.654
7.635
7.615
7.521
7.503
7.501
7.482
5.244
5.229
5.213
5.197
5.182
1.268
1.252
3ja
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.998
1.041
1.058
1.187
1.124
1.155
1.029
1.076
1.060
1.111
6.411


170.707
161.873
159.365
157.839
156.780
135.185
132.500
130.939
129.222
128.817
128.059
126.770
126.326
125.427
124.669
119.120
69.692
21.645
3ja
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.276
8.709
8.697
8.298
8.278
8.061
8.042
8.040
7.921
7.917
7.901
7.897
7.892
7.882
7.878
7.871
7.667
7.652
7.541
7.519
7.502
7.487
7.421
7.401
5.111
5.095
5.080
5.064
5.048
2.474
1.195
1.179
3ka
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.118
1.087
1.086
2.114
1.019
2.082
0.935
1.116
2.908
5.962


170.356
169.257
163.620
149.929
148.085
145.240
137.534
129.935
129.670
128.550
128.169
126.788
126.631
126.434
125.240
124.630
122.853
118.859
69.678
21.522
21.071
3ka
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.550
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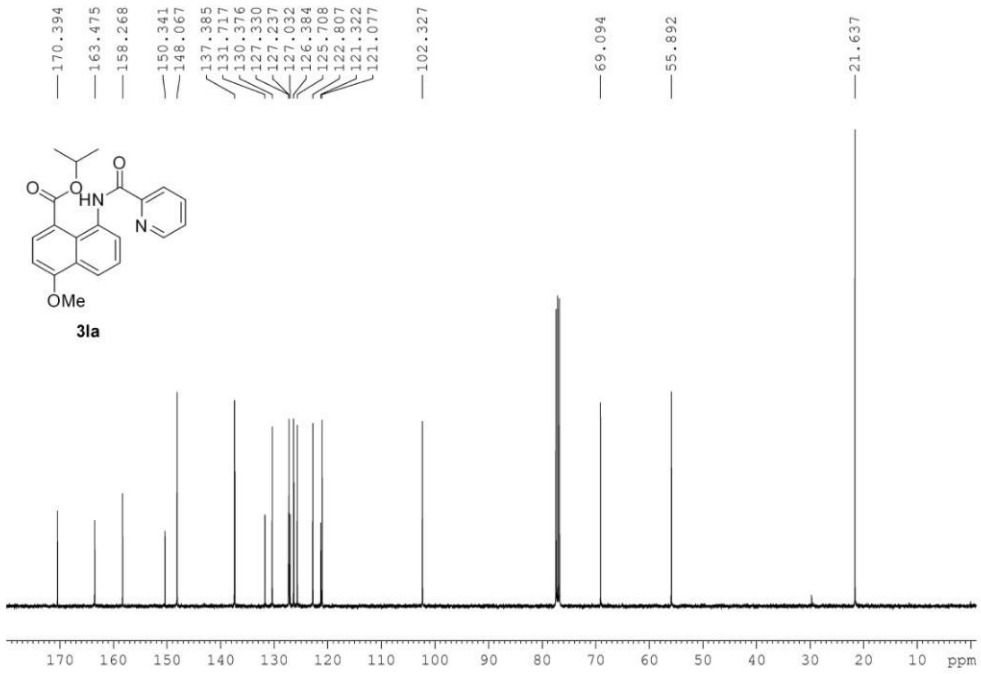
8.689
8.311
8.290
8.277
8.258
7.974
7.956
7.886
7.866
7.847
7.734
7.713
7.626
7.606
7.586
7.480
7.468
7.465
7.461
7.449
7.767
6.747
5.187
5.171
5.156
5.140
5.124
4.003
1.221
1.206
OMe
3la
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.023
2.010
0.970
1.011
0.987
1.015
0.994
1.017
1.007
3.044
6.064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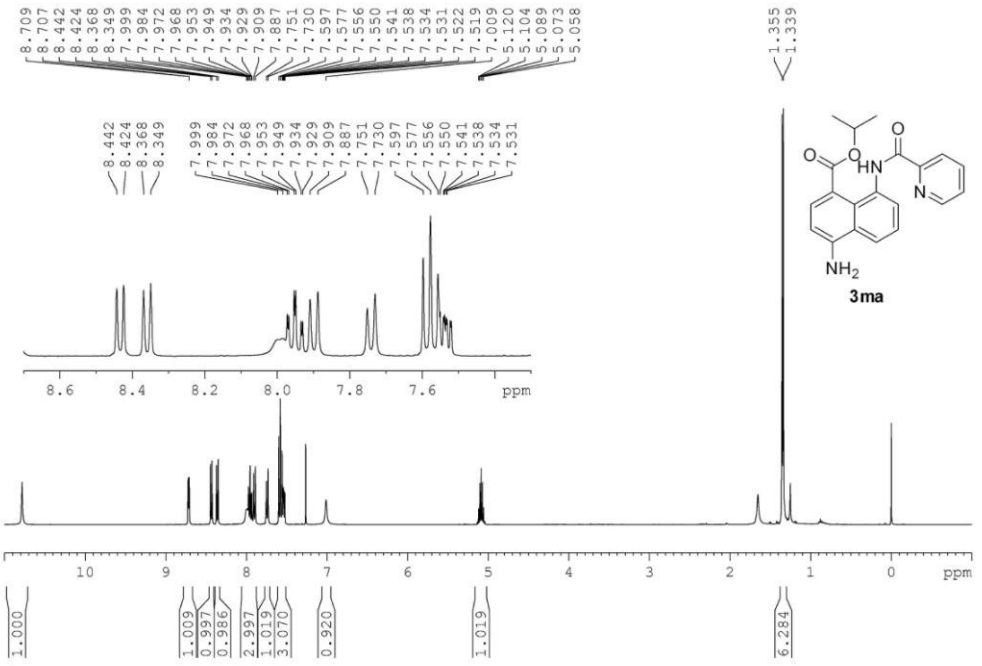
163.475
158.268
150.341
148.067
137.385
131.717
130.376
127.330
127.237
127.032
126.384
125.708
122.807
121.322
121.077
102.327
69.094
55.892
21.637
OMe
3la
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.707
8.442
8.424
8.368
8.349
7.999
7.984
7.972
7.968
7.953
7.949
7.934
7.929
7.909
7.887
7.751
7.730
7.597
7.577
7.556
7.550
7.541
7.538
7.534
7.531
7.522
7.519
7.009
5.120
5.104
5.089
5.073
5.058
1.355
1.339
NH2
3ma
8.6 8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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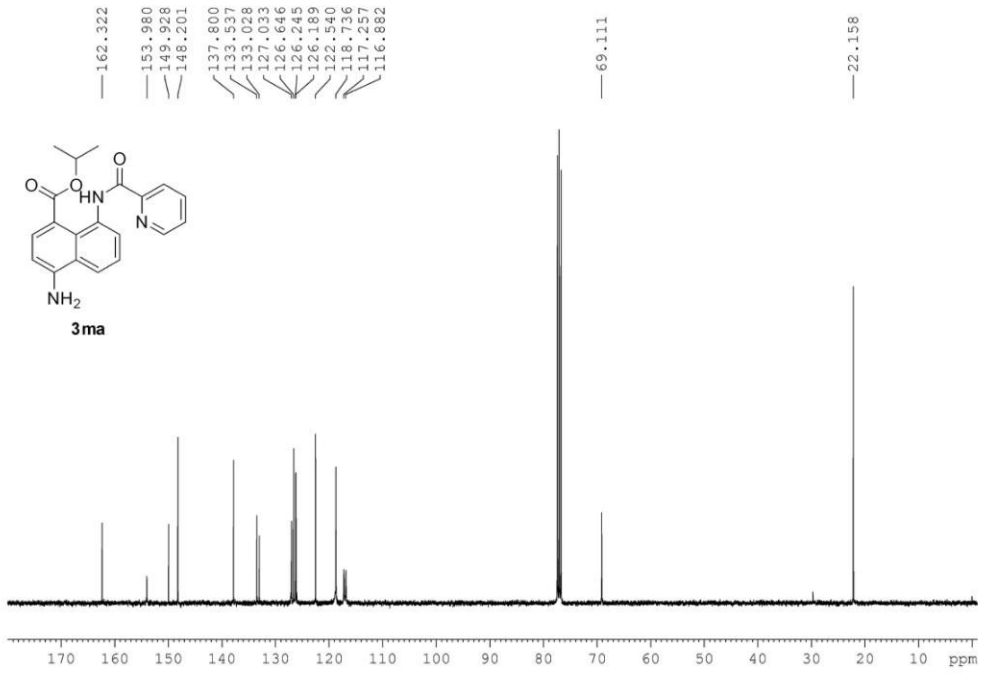
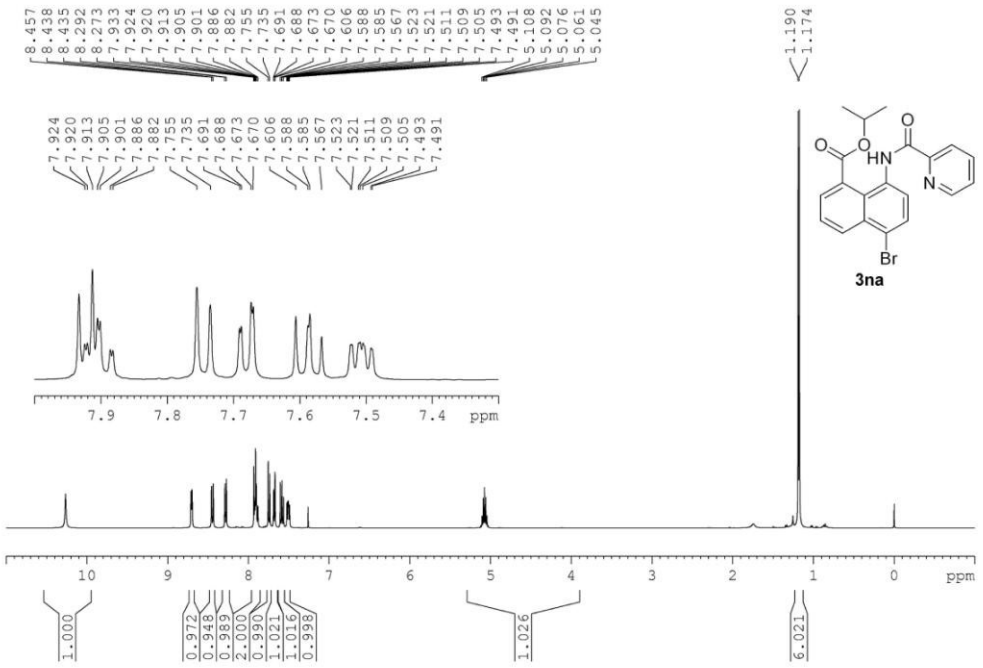
0.997
0.986
2.997
1.019
3.070
0.920
1.019
6.284


162.322
153.980
149.928
148.201
137.800
133.537
133.028
127.033
126.646
126.245
126.189
122.540
118.736
117.257
116.882
69.111
22.158
3ma
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.438
8.435
8.292
8.273
7.933
7.924
7.920
7.913
7.905
7.901
7.886
7.882
7.755
7.735
7.691
7.688
7.673
7.670
7.606
7.588
7.585
7.567
7.523
7.521
7.511
7.509
7.505
7.493
7.491
5.108
5.092
5.076
5.061
5.045
1.190
1.174
3na
7.9 7.8 7.7 7.6 7.5 7.4 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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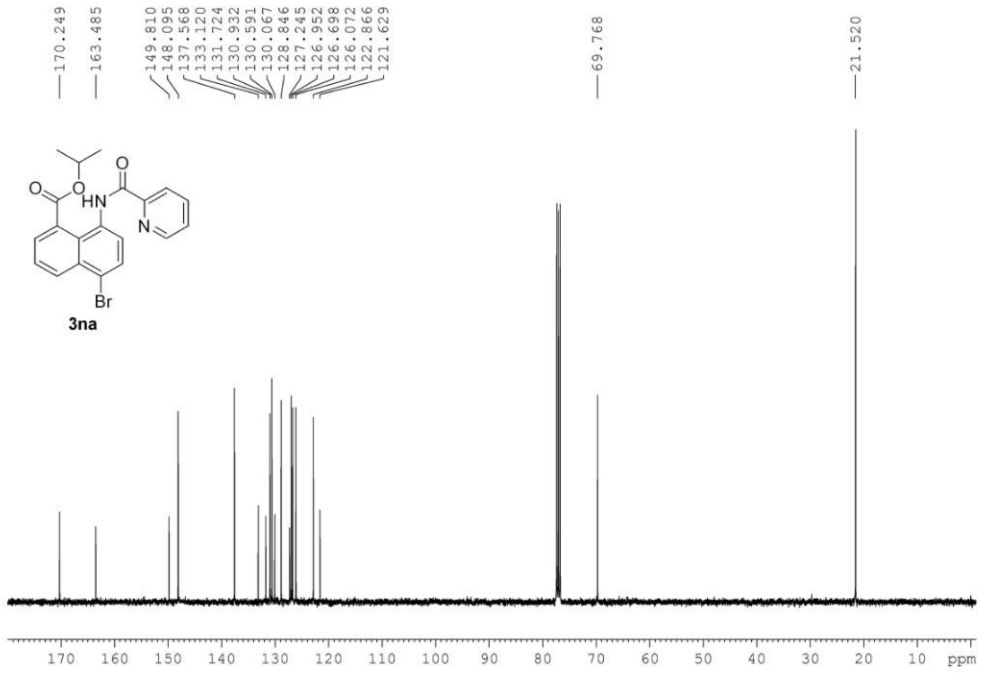
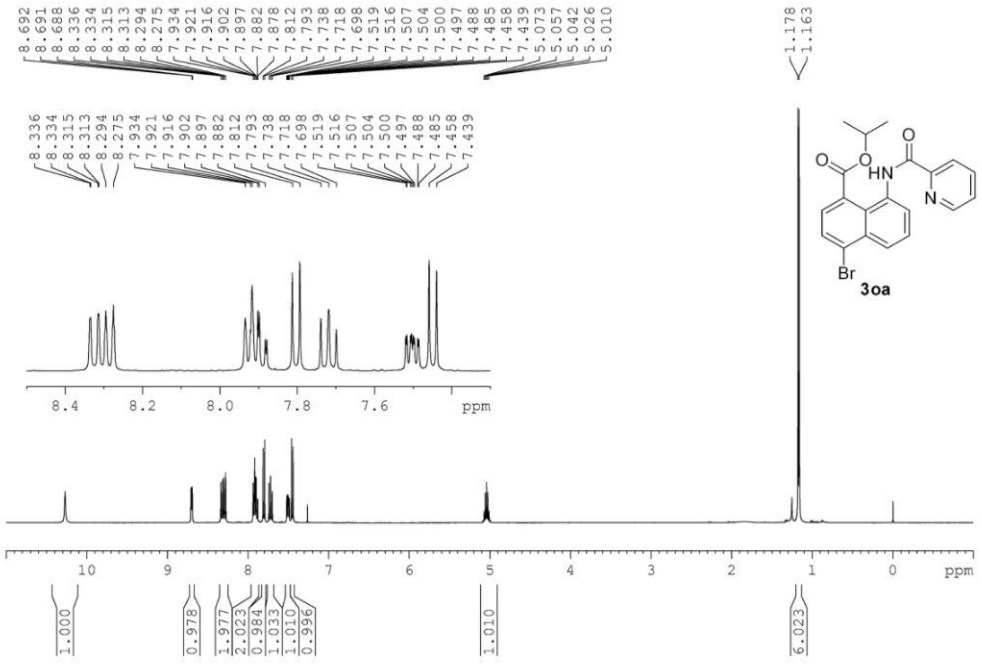
0.948
0.989
2.000
0.990
1.021
1.016
0.998
1.026
6.021


170.249
163.485
149.810
148.095
137.568
133.120
131.724
130.932
130.591
130.067
128.846
127.245
126.952
126.698
126.072
122.866
121.629
69.768
21.520
3na
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.688
8.336
8.334
8.315
8.313
8.294
8.275
7.934
7.921
7.916
7.902
7.897
7.882
7.878
7.812
7.793
7.738
7.718
7.698
7.519
7.516
7.507
7.504
7.500
7.497
7.488
7.485
7.458
7.439
5.073
5.057
5.042
5.026
5.010
1.178
1.163
3oa
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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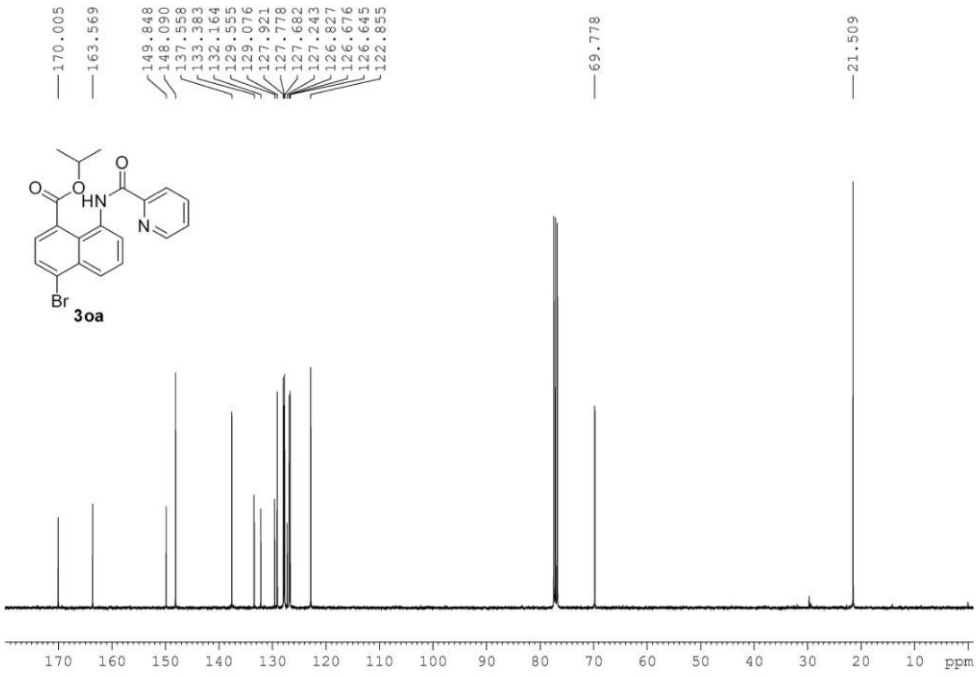
0.978
1.977
2.023
0.984
1.033
1.010
0.996
1.010
6.023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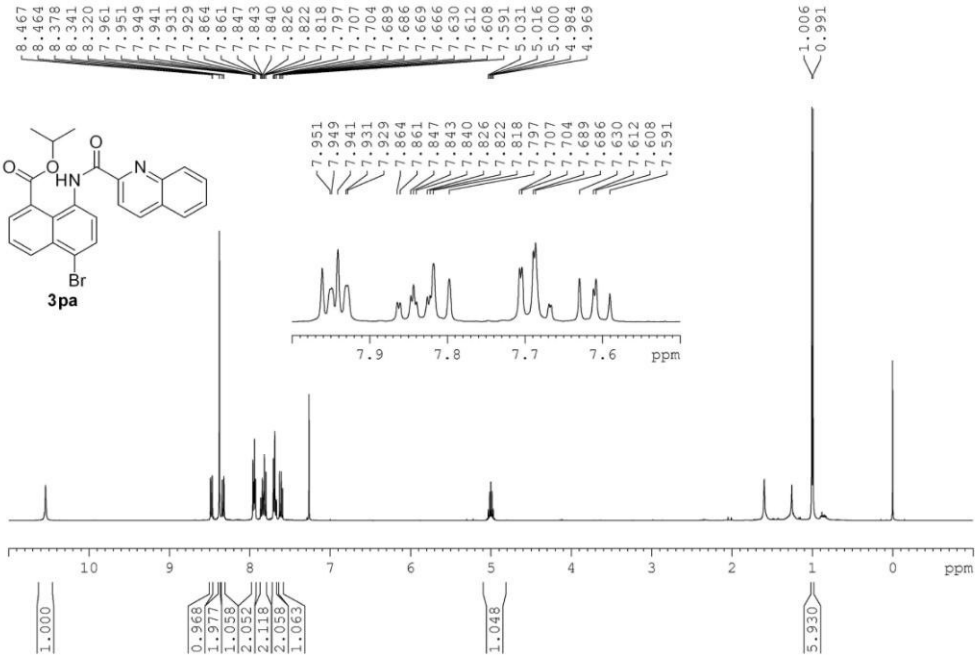
163.569
149.848
148.090
137.558
133.383
132.164
129.555
129.076
127.921
127.778
127.682
127.243
126.827
126.676
126.645
122.855
69.778
21.509
3oa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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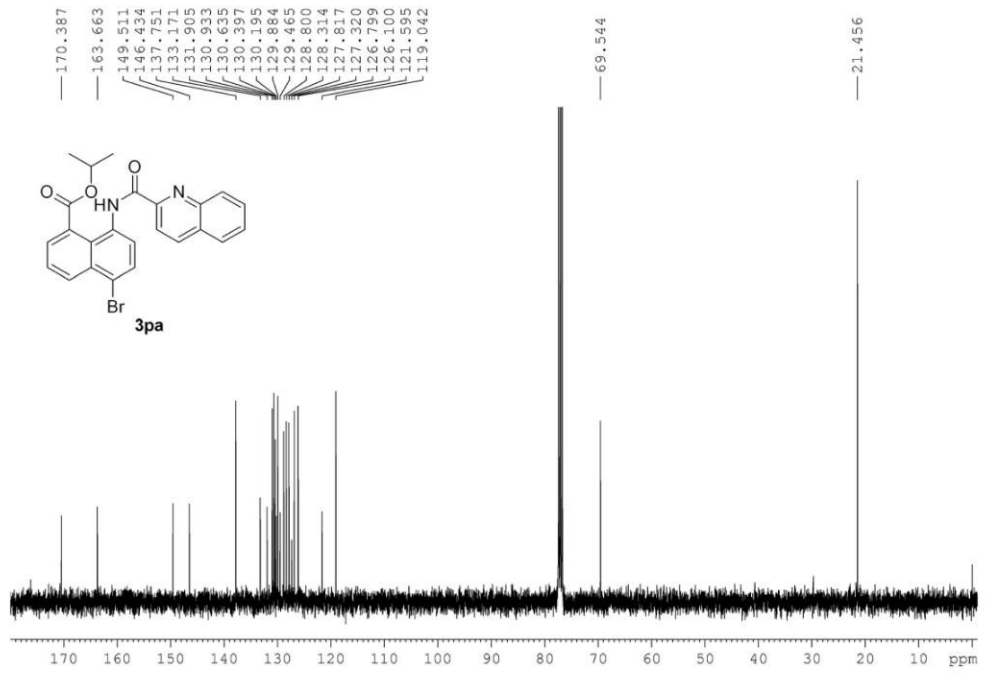
8.464
8.378
8.341
8.320
7.961
7.951
7.949
7.941
7.931
7.929
7.864
7.861
7.847
7.843
7.840
7.826
7.822
7.818
7.797
7.707
7.704
7.689
7.686
7.669
7.666
7.630
7.612
7.608
7.591
5.031
5.016
5.000
4.984
4.969
1.006
0.991
3pa
7.9 7.8 7.7 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.968
1.977
1.058
2.052
2.118
2.058
1.063
1.048
5.930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149.511
146.434
137.751
133.171
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130.933
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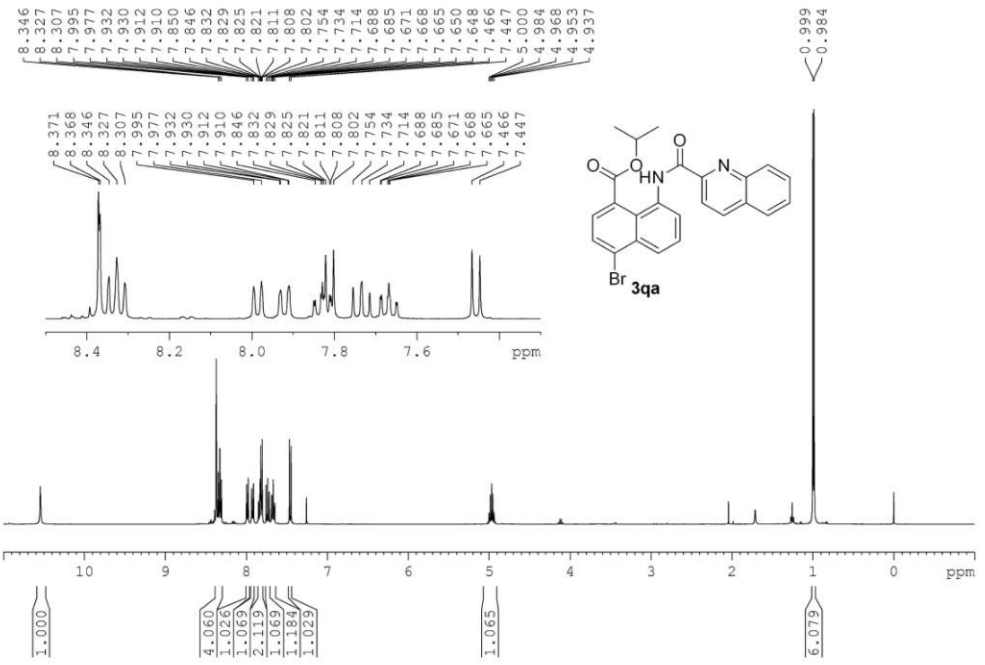
130.397
130.195
129.884
129.465
128.800
128.314
127.817
127.320
126.799
126.100
121.595
119.042
69.544
21.456
O
O
HN
N
Br
3pa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.327
8.307
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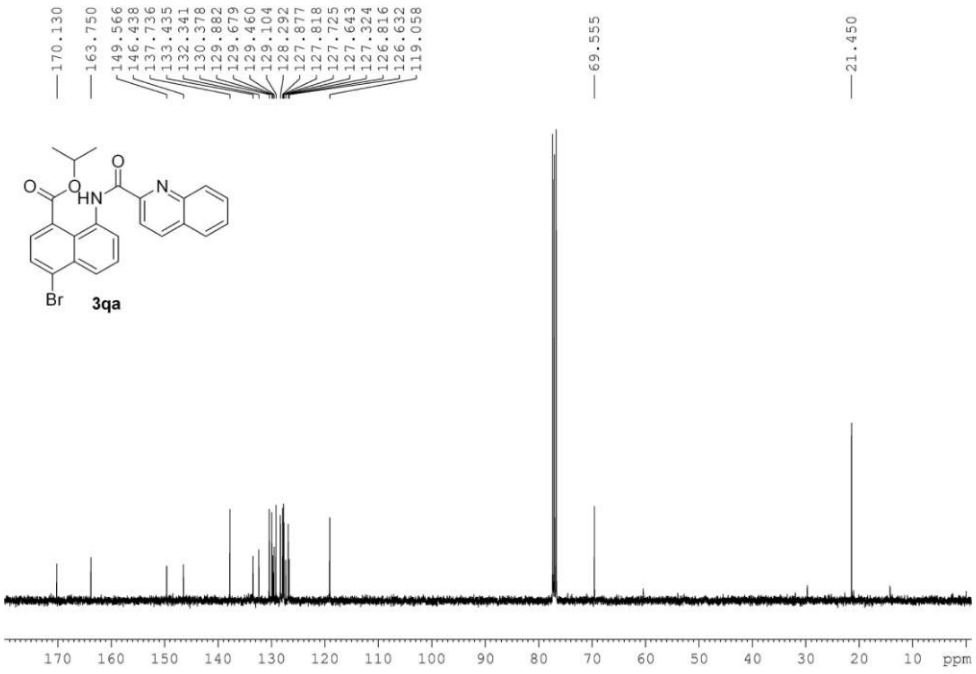
7.930
7.912
7.910
7.850
7.846
7.832
7.829
7.825
7.821
7.811
7.808
7.802
7.754
7.734
7.714
7.688
7.685
7.671
7.668
7.665
7.650
7.648
7.466
7.447
5.000
4.984
4.968
4.953
4.937
0.999
0.984
O
O
HN
N
Br
3qa
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
4.060
1.026
1.069
2.119
1.069
1.184
1.029
1.065
6.079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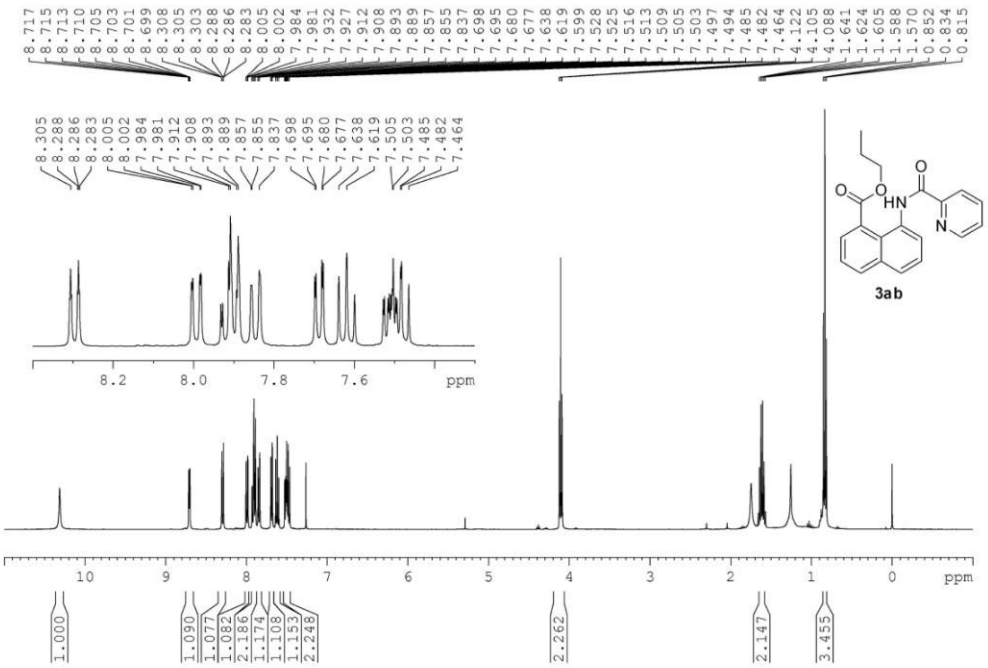
149.566
146.438
137.736
133.435
132.341
130.378
129.882
129.679
129.460
129.104
128.292
127.877
127.818
127.725
127.643
127.324
126.816
126.632
119.058
69.555
21.450
3qa
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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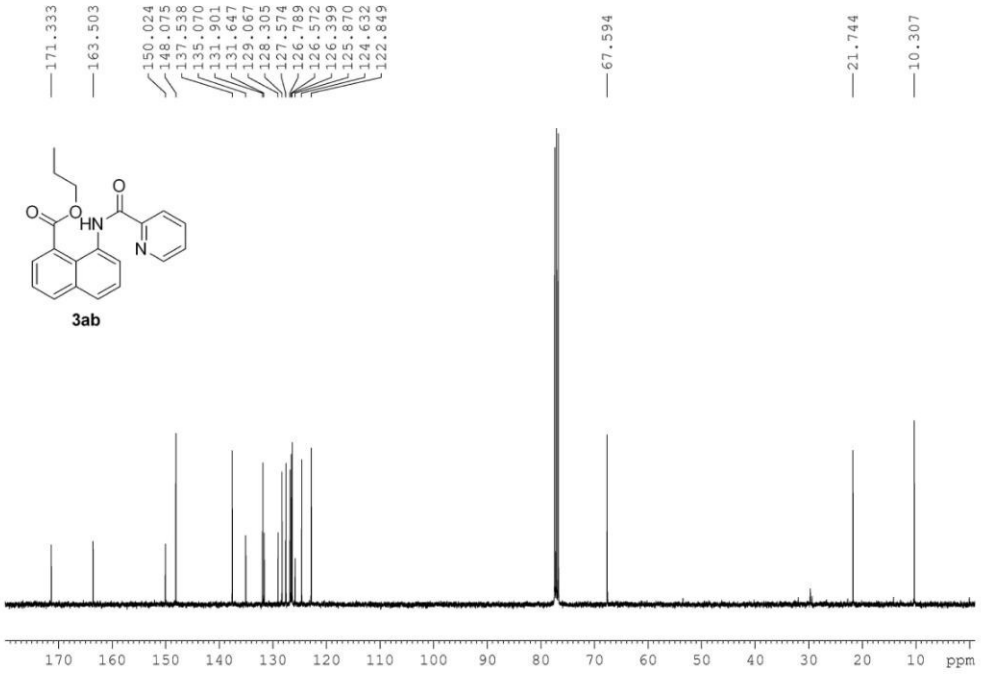
8.715
8.713
8.710
8.705
8.703
8.701
8.699
8.308
8.305
8.303
8.288
8.286
8.283
8.005
8.002
7.984
7.981
7.932
7.927
7.912
7.908
7.893
7.889
7.857
7.855
7.837
7.698
7.695
7.680
7.677
7.638
7.619
7.599
7.528
7.525
7.516
7.513
7.509
7.505
7.503
7.497
7.494
7.485
7.482
7.464
4.122
4.105
4.088
1.641
1.624
1.605
1.588
1.570
0.852
0.834
0.815
3ab
8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.090
1.077
1.082
2.186
1.174
1.108
1.153
2.248
2.262
2.147
3.455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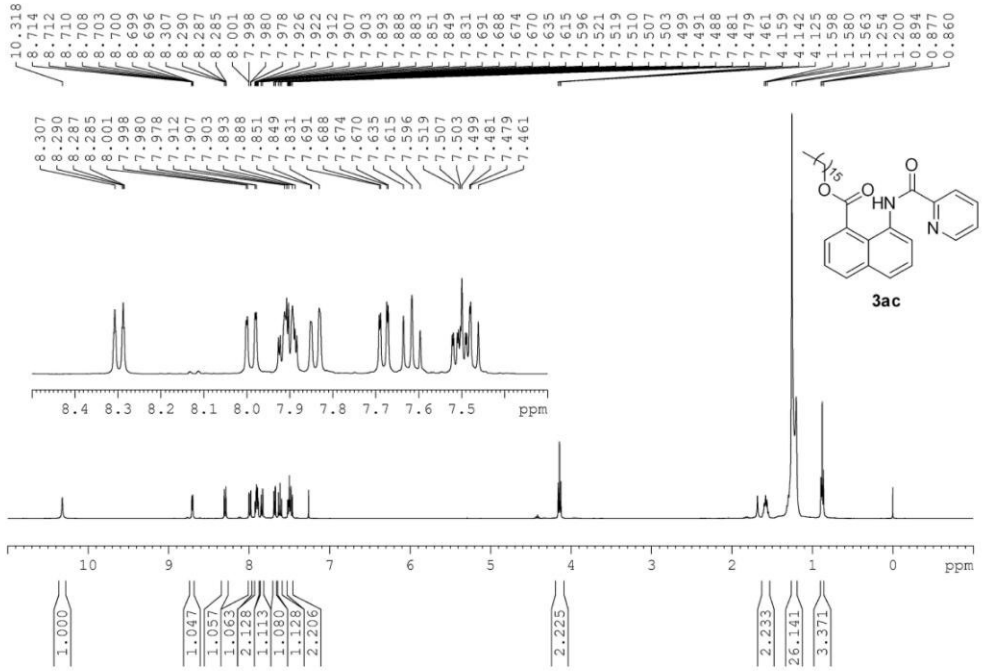
163.503
150.024
148.075
137.538
135.070
131.901
131.647
129.067
128.305
127.574
126.789
126.572
126.399
125.870
124.632
122.849
67.594
21.744
10.307
3ab
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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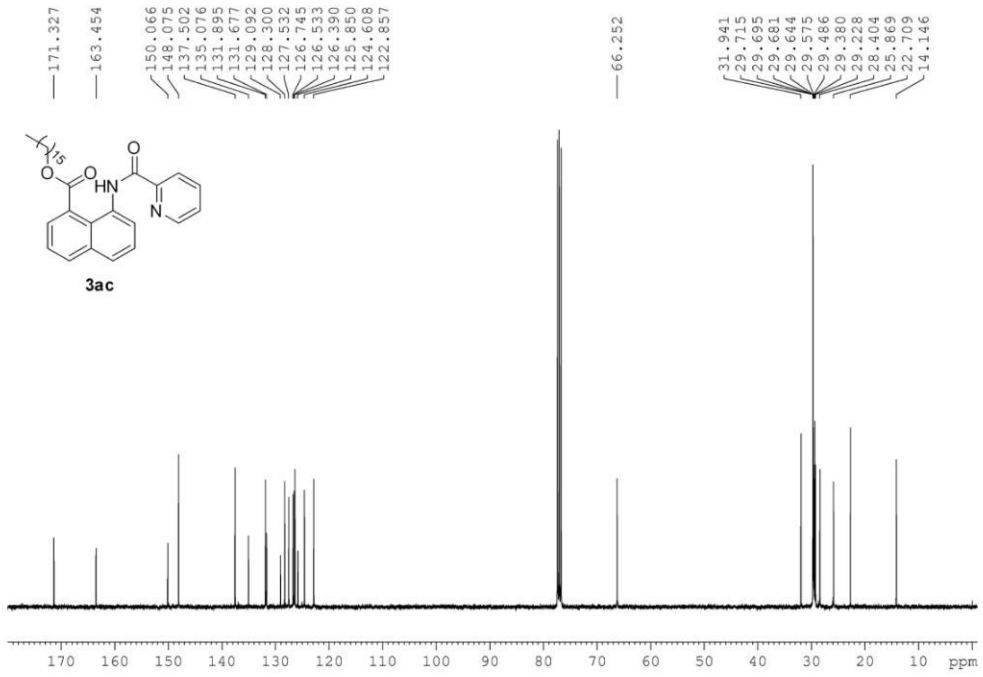
8.714
8.712
8.710
8.708
8.703
8.700
8.699
8.696
8.307
8.290
8.287
8.285
8.001
7.998
7.980
7.978
7.926
7.922
7.912
7.907
7.903
7.893
7.888
7.883
7.851
7.849
7.831
7.691
7.688
7.674
7.670
7.635
7.615
7.596
7.521
7.519
7.510
7.507
7.503
7.499
7.491
7.488
7.481
7.479
7.461
4.159
4.142
4.125
1.598
1.580
1.563
1.254
1.200
0.894
0.877
0.860
3ac
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.047
1.057
1.063
2.128
1.113
1.080
1.128
2.206
2.225
2.233
26.141
3.371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163.454
150.066
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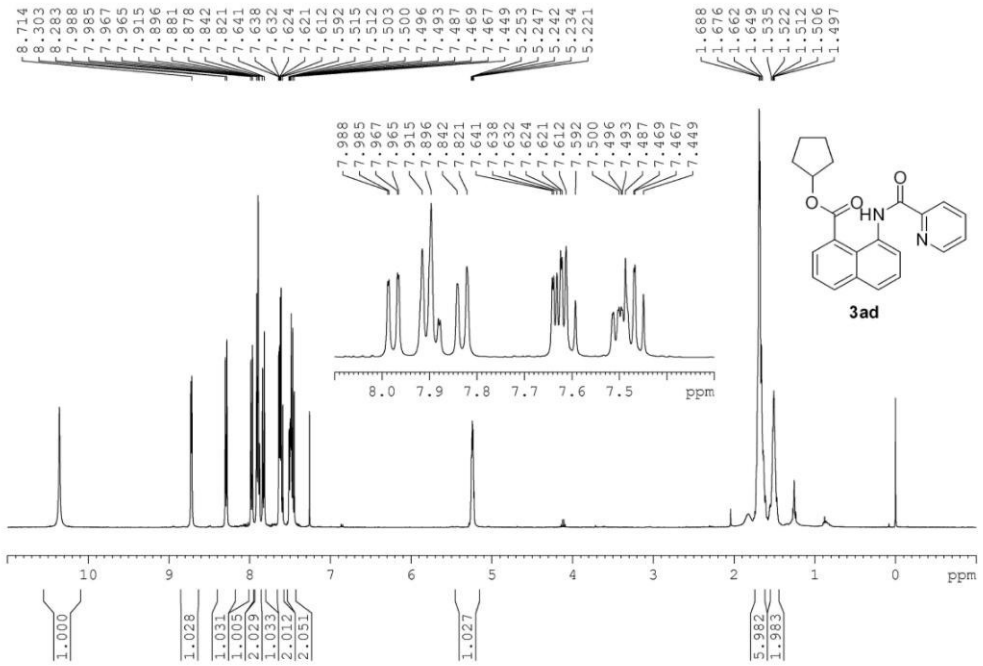
137.502
135.076
131.895
131.677
129.092
128.300
127.532
126.745
126.533
126.390
125.850
124.608
122.857
66.252
31.941
29.715
29.695
29.681
29.644
29.575
29.486
29.380
29.228
28.404
25.869
22.709
14.146
3ac
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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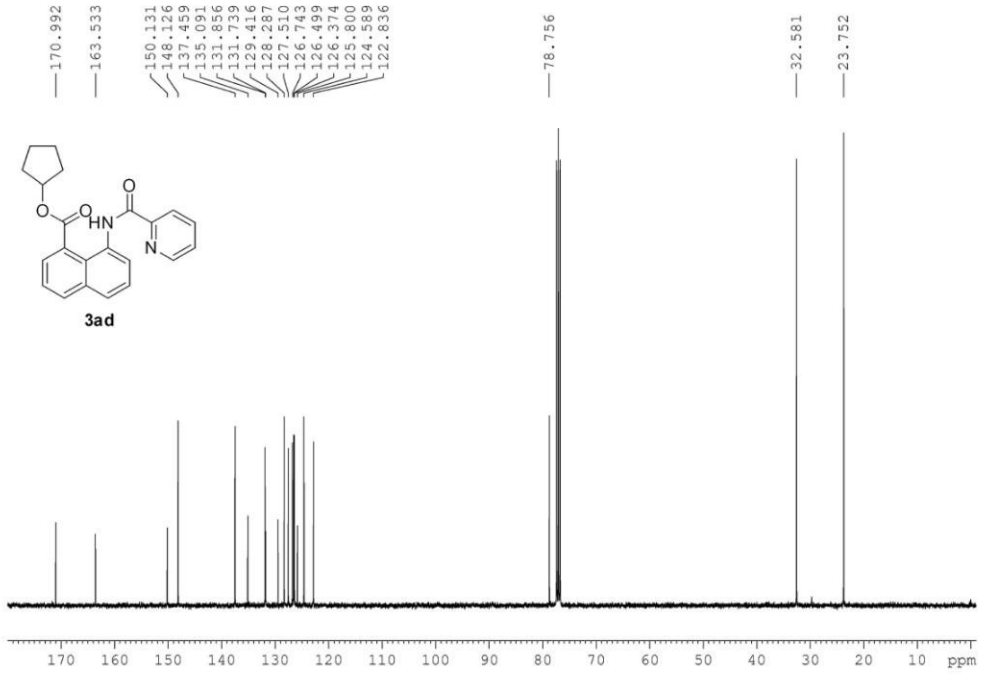
8.303
8.283
7.988
7.985
7.967
7.965
7.915
7.896
7.881
7.878
7.842
7.821
7.641
7.638
7.632
7.624
7.621
7.612
7.592
7.515
7.512
7.503
7.500
7.496
7.493
7.487
7.469
7.467
7.449
5.253
5.247
5.242
5.234
5.221
1.688
1.676
1.662
1.649
1.535
1.522
1.512
1.506
1.497
3ad
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.028
1.031
1.005
2.029
1.033
2.012
2.051
1.027
5.982
1.983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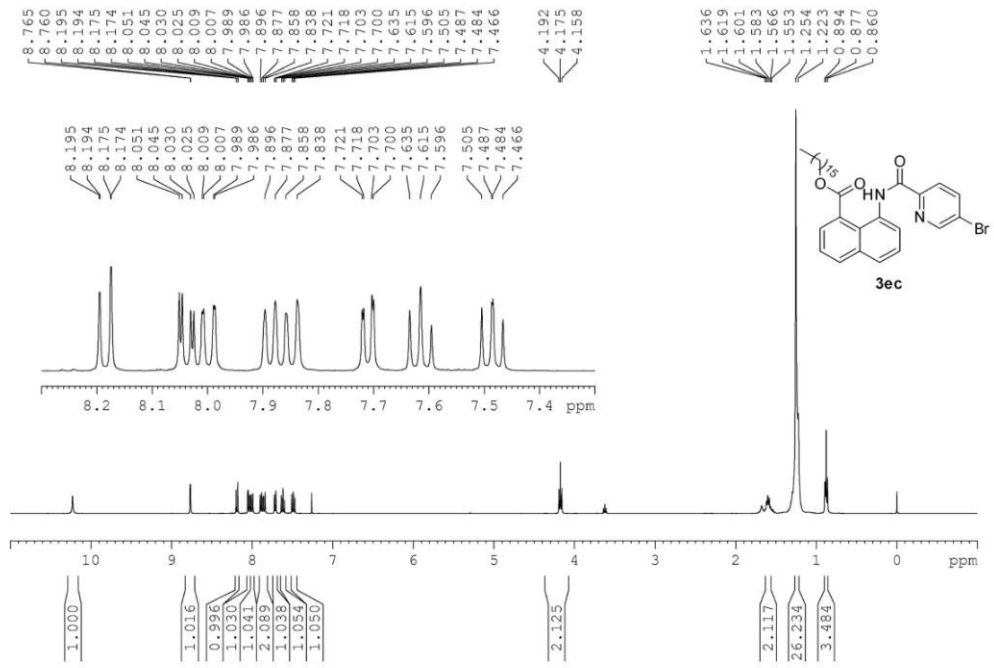
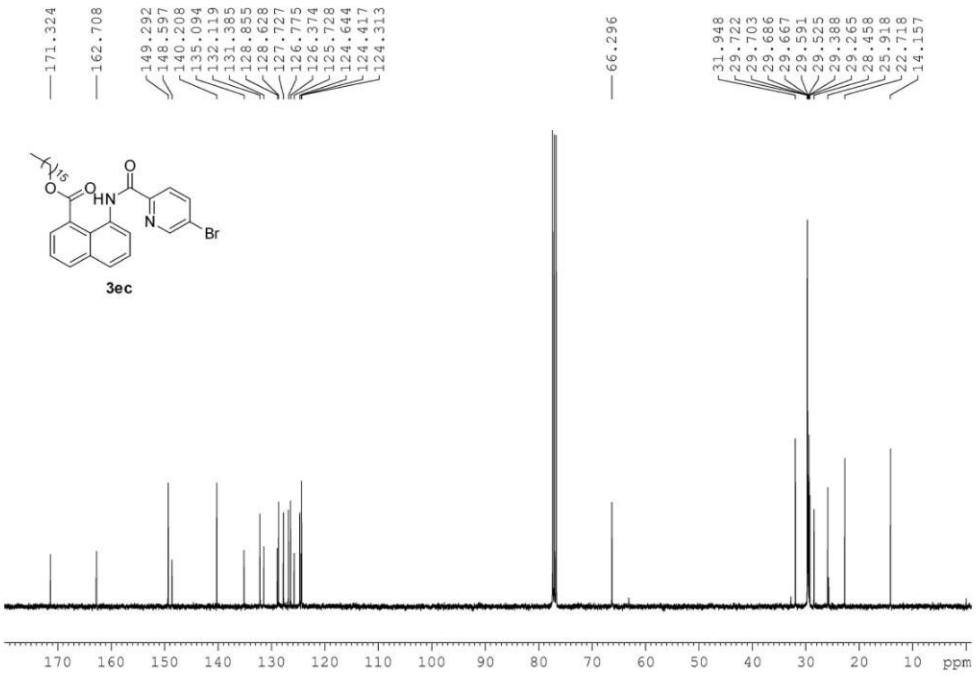
150.131
148.126
137.459
135.091
131.856
131.739
129.416
128.287
127.510
126.743
126.499
126.374
125.800
124.589
122.836
78.756
32.581
23.752
3ad
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.765
8.760
8.195
8.194
8.175
8.174
8.051
8.045
8.030
8.025
8.009
8.007
7.989
7.986
7.896
7.877
7.858
7.838
7.721
7.718
7.703
7.700
7.635
7.615
7.596
7.505
7.487
7.484
7.466
4.192
4.175
4.158
1.636
1.619
1.601
1.583
1.566
1.553
1.254
1.223
0.894
0.877
0.860
3ec
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.016
0.996
1.030
1.041
2.089
1.038
1.054
1.050
2.125
2.117
26.234
3.484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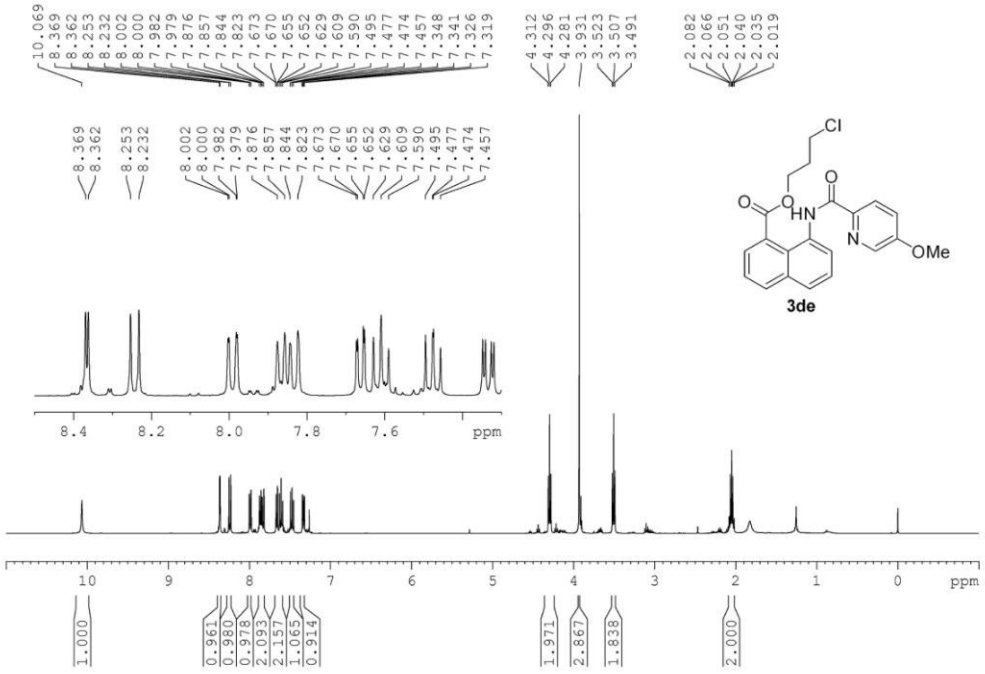
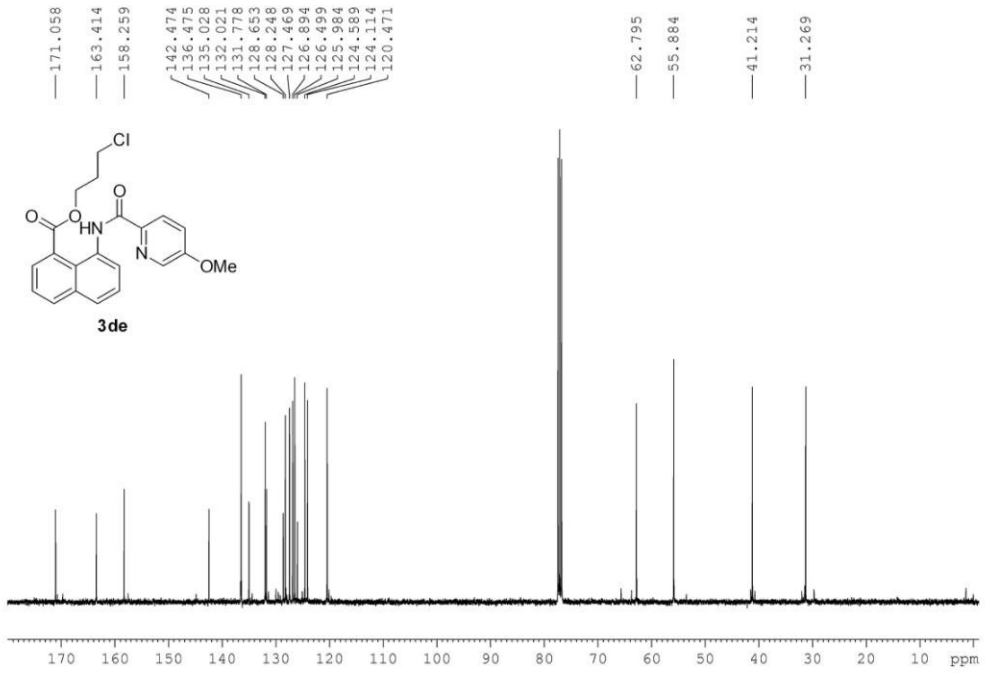
162.708
149.292
148.597
140.208
135.094
132.119
131.385
128.855
128.628
127.727
126.775
126.374
125.728
124.644
124.417
124.313
66.296
31.948
29.722
29.703
29.686
29.667
29.591
29.525
29.388
29.265
28.458
25.918
22.718
14.157
3ec
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.069
8.369
8.362
8.253
8.232
8.002
8.000
7.982
7.979
7.876
7.857
7.844
7.823
7.673
7.670
7.655
7.652
7.629
7.609
7.590
7.495
7.477
7.474
7.457
7.348
7.341
7.326
7.319
4.312
4.296
4.281
3.931
3.523
3.507
3.491
2.082
2.066
2.051
2.040
2.035
2.019
3de
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.961
0.980
0.978
2.093
2.157
1.065
0.914
1.971
2.867
1.838
2.000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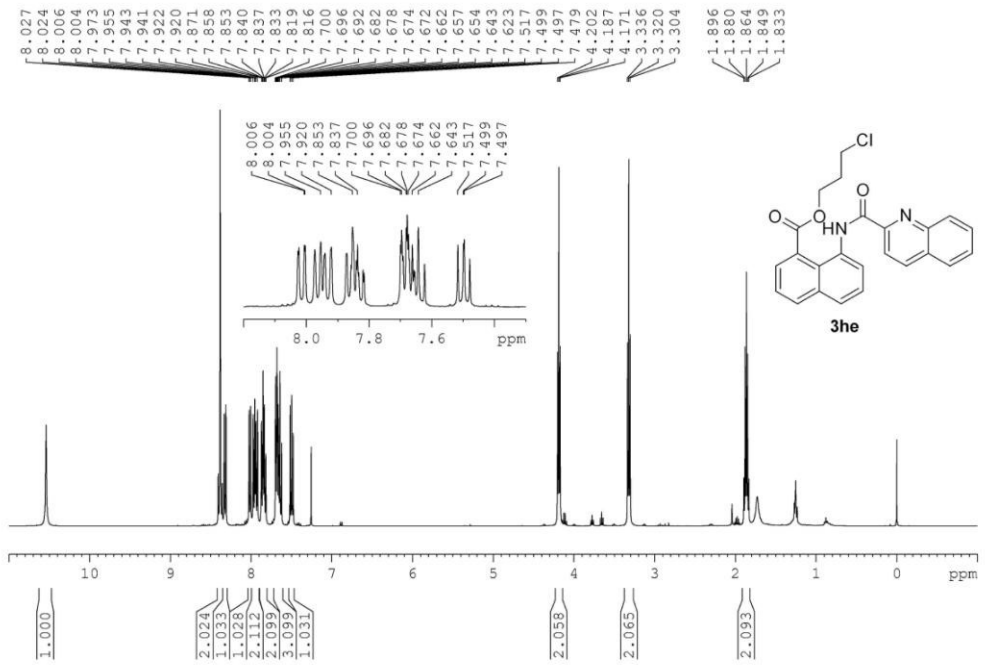
163.414
158.259
142.474
136.475
135.028
132.021
131.778
128.653
128.248
127.469
126.894
126.499
125.984
124.589
124.114
120.471
62.795
55.884
41.214
31.269
Cl
O
O
HN
N
OMe
3de
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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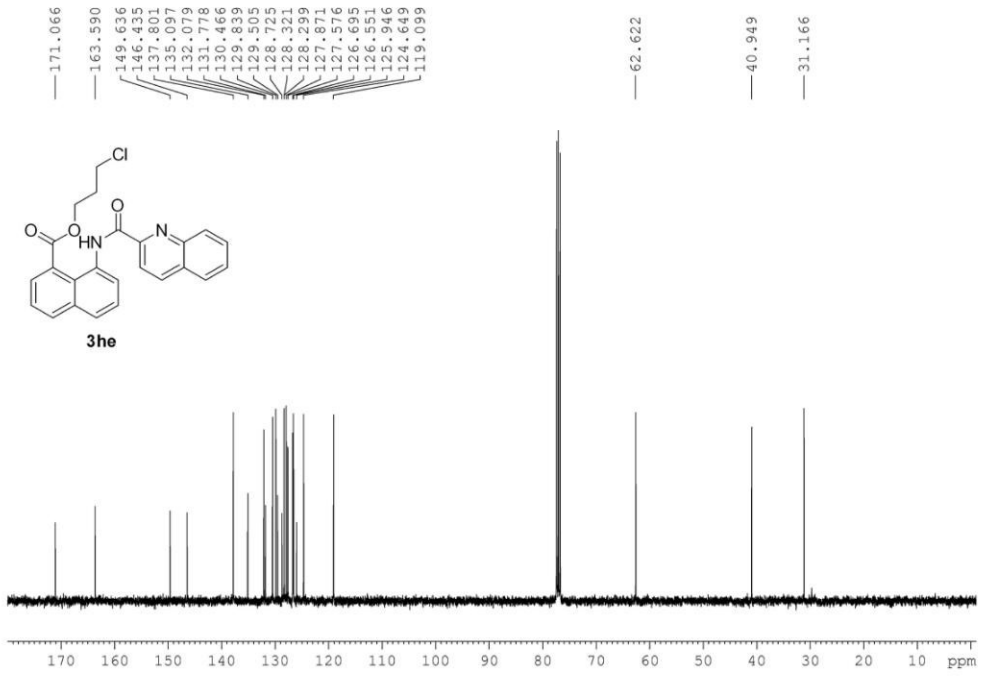
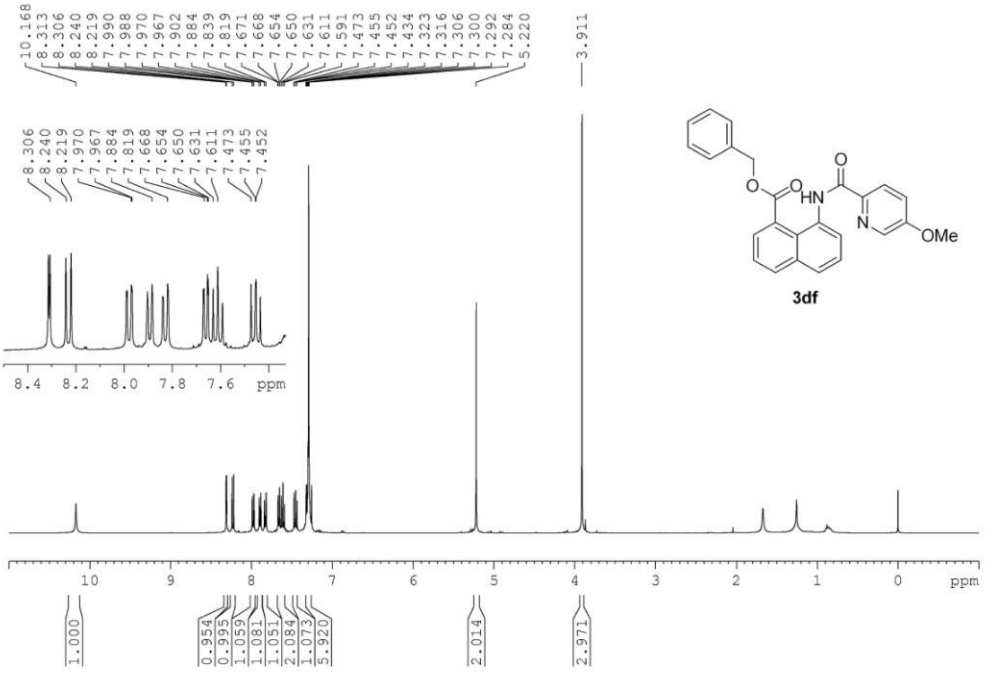
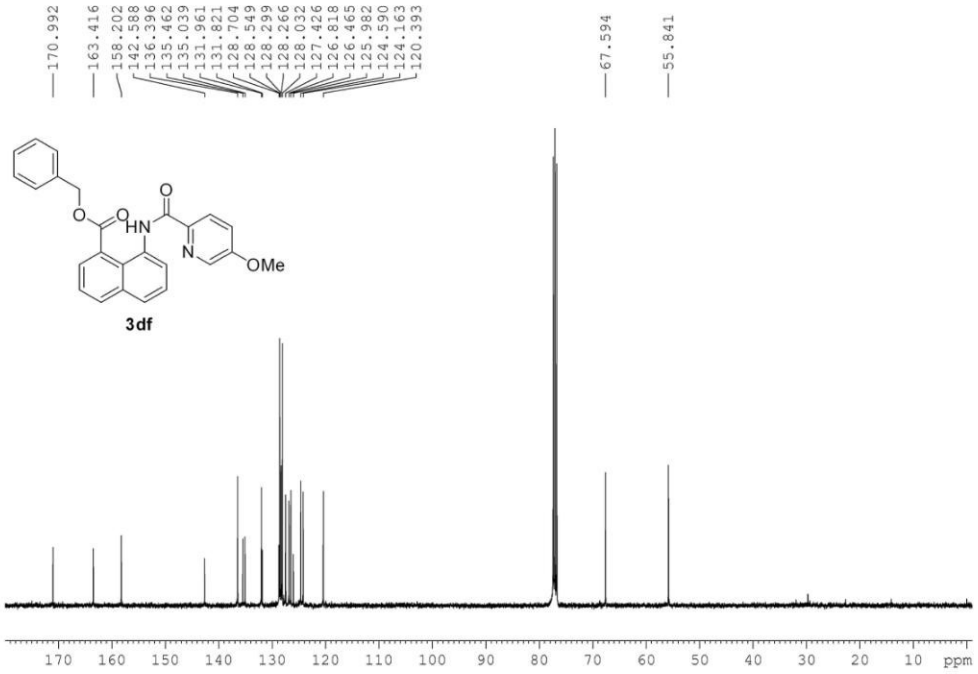
8.024
8.006
8.004
7.973
7.955
7.943
7.941
7.922
7.920
7.871
7.858
7.853
7.840
7.837
7.833
7.819
7.816
7.700
7.696
7.692
7.682
7.678
7.674
7.672
7.662
7.657
7.654
7.643
7.623
7.517
7.499
7.497
7.479
4.202
4.187
4.171
3.336
3.320
3.304
1.896
1.880
1.864
1.849
1.833
8.0 7.8 7.6 ppm
Cl
O
O
HN
N
3he
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
2.024
1.033
1.028
2.112
2.099
2.099
3.099
1.031
2.058
2.065
2.093


171.066
163.590
149.636
146.435
137.801
135.097
132.079
131.778
130.466
129.839
129.505
128.725
128.321
128.299
127.871
127.576
126.695
126.551
125.946
124.649
119.099
62.622
40.949
31.166
Cl
O
O
HN
O
N
3he
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.168
8.313
8.306
8.240
8.219
7.990
7.988
7.970
7.967
7.902
7.884
7.839
7.819
7.671
7.668
7.654
7.650
7.631
7.611
7.591
7.473
7.455
7.452
7.434
7.323
7.316
7.306
7.300
7.292
7.284
5.220
3.911
8.4 8.2 8.0 7.8 7.6 ppm
O
O
HN
N
OMe
3df
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.954
0.995
1.059
1.081
1.051
2.084
1.073
5.920
2.014
2.971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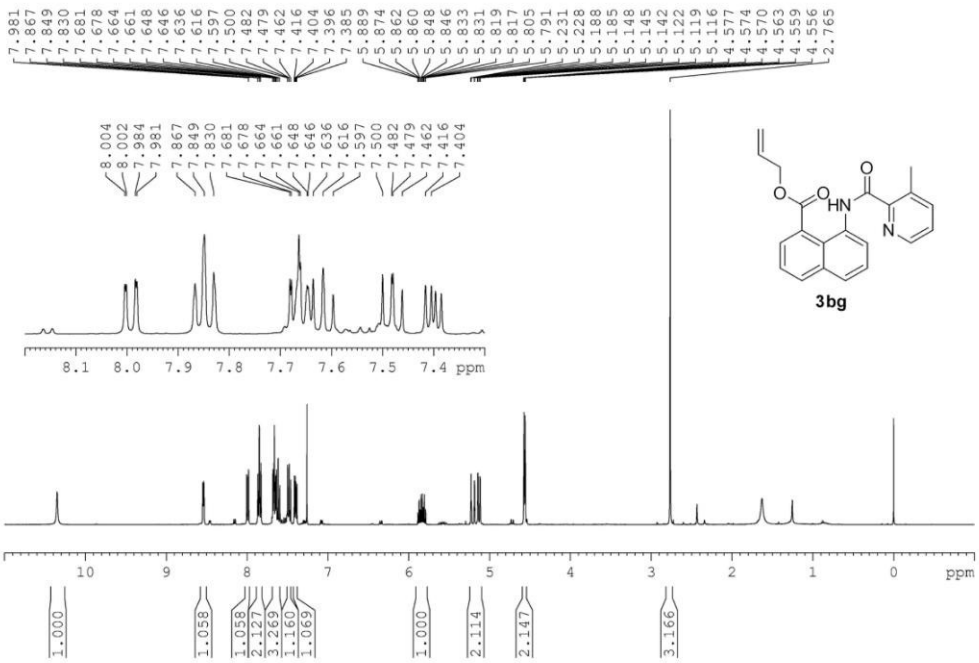
163.416
158.202
142.588
136.396
135.462
135.039
131.961
131.821
128.704
128.549
128.299
128.266
128.032
127.426
126.818
126.465
125.982
124.590
124.163
120.393
67.594
55.841
O
O
HN
O
N
OMe
3df
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.981
7.867
7.849
7.830
7.681
7.678
7.664
7.661
7.648
7.646
7.636
7.616
7.597
7.500
7.482
7.479
7.462
7.416
7.404
7.396
7.385
5.889
5.874
5.862
5.860
5.848
5.846
5.833
5.831
5.819
5.817
5.805
5.791
5.231
5.228
5.188
5.185
5.148
5.145
5.142
5.122
5.119
5.116
4.577
4.574
4.570
4.563
4.559
4.556
2.765
O
O
HN
O
N
3bg
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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1.058
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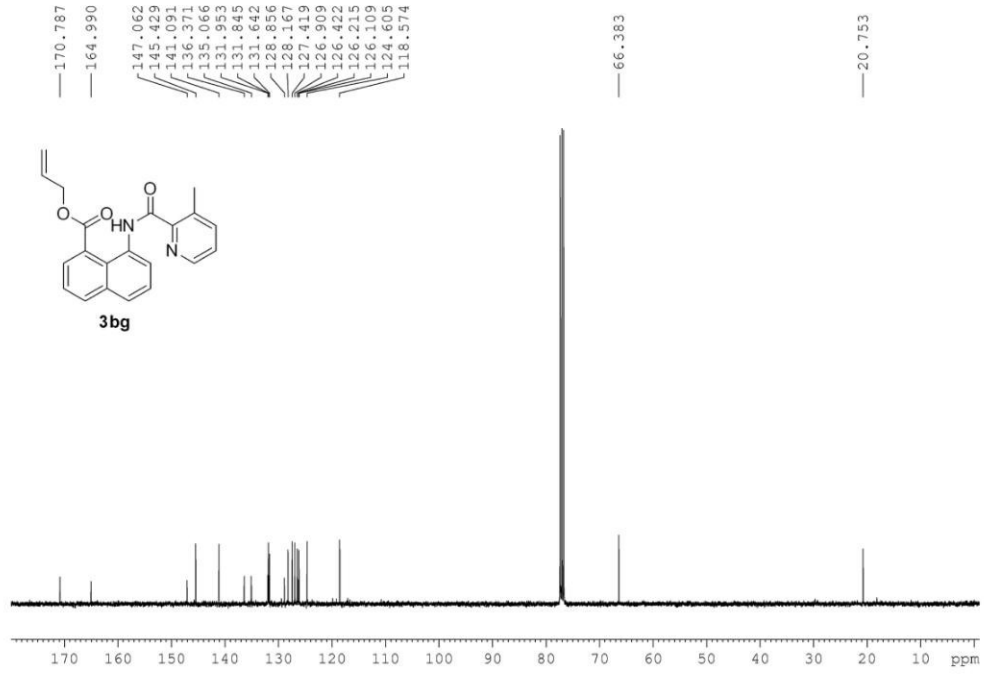
3.269
1.160
1.069
1.000
2.114
2.147
3.166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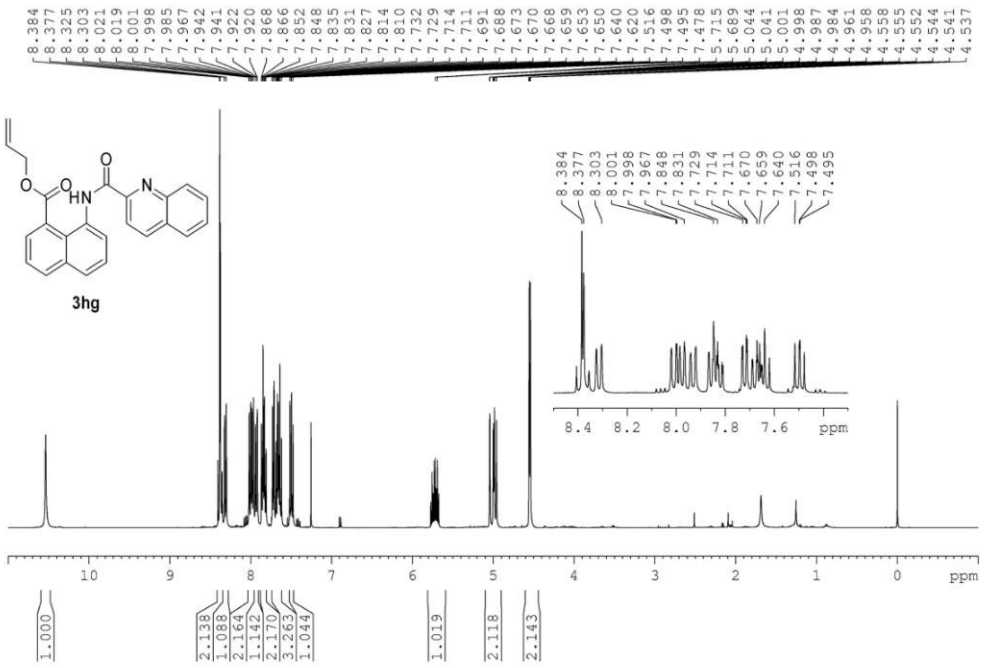
145.429
141.091
136.371
135.066
131.953
131.845
131.642
128.856
128.167
127.419
126.909
126.422
126.215
126.109
124.605
118.574
66.383
20.753
3bg
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.303
8.021
8.019
8.001
7.998
7.985
7.967
7.942
7.941
7.922
7.920
7.868
7.866
7.852
7.848
7.835
7.831
7.827
7.814
7.810
7.732
7.729
7.714
7.711
7.691
7.688
7.673
7.670
7.668
7.659
7.653
7.650
7.640
7.620
7.516
7.498
7.495
7.478
5.715
5.689
5.044
5.041
5.001
4.998
4.987
4.984
4.961
4.958
4.558
4.555
4.552
4.544
4.541
4.537
3hg
8.4 8.2 8.0 7.8 7.6 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
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1.088
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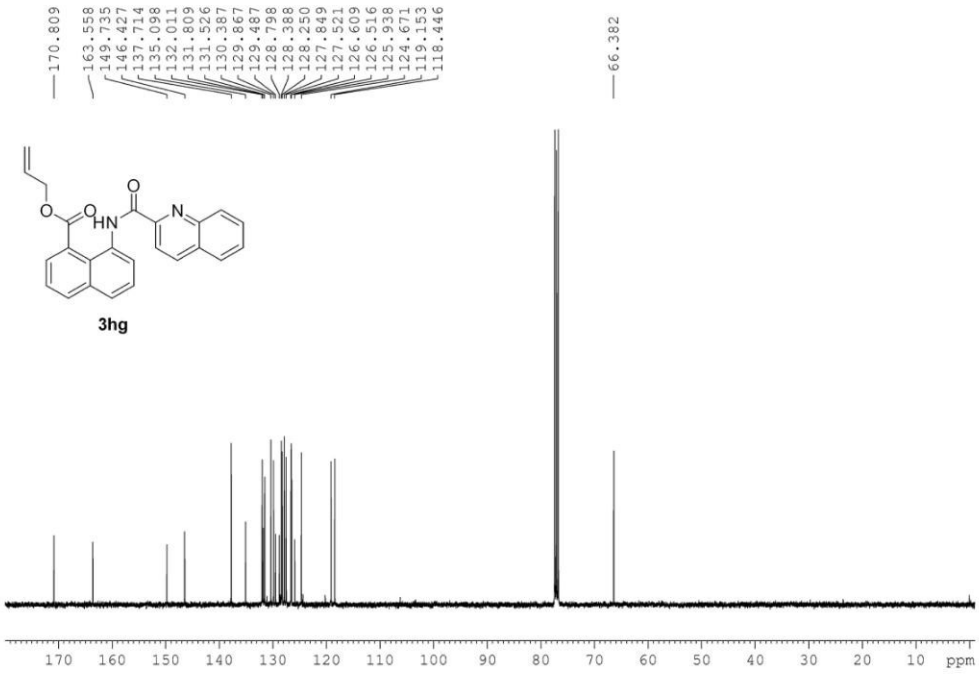
1.142
2.170
3.263
1.044
1.019
2.118
2.143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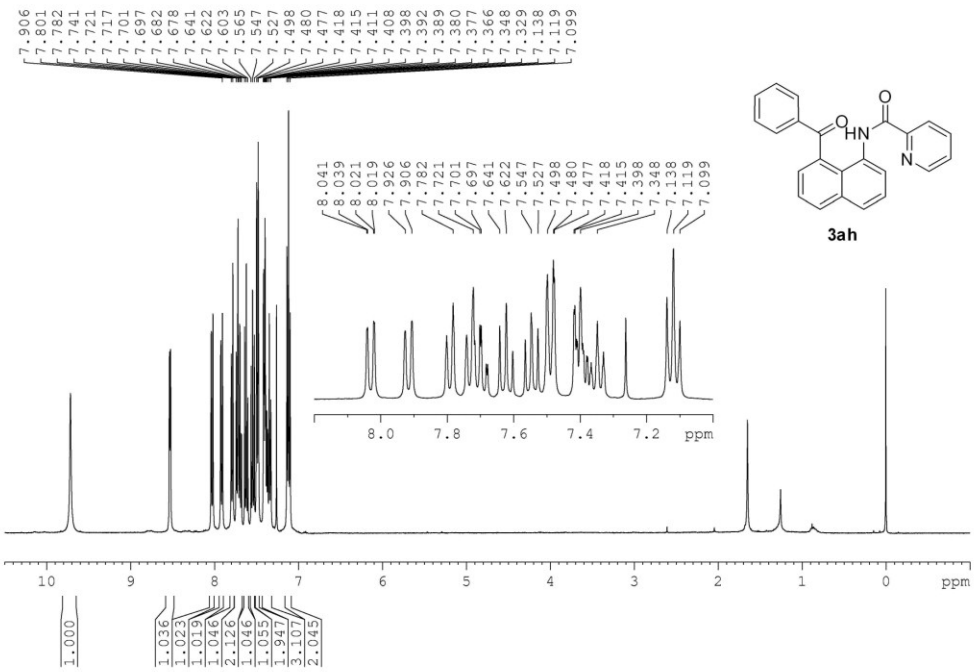
146.427
137.714
135.098
132.011
131.809
131.526
130.387
129.867
129.487
128.798
128.388
128.250
127.849
127.521
126.609
126.516
125.938
124.671
119.153
118.446
66.382
3hg
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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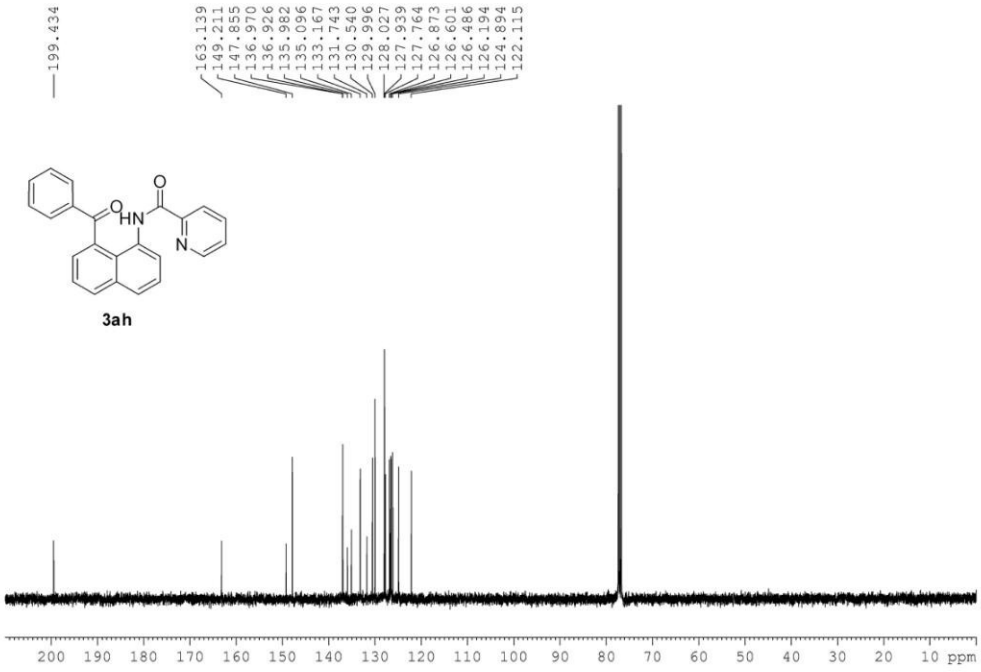
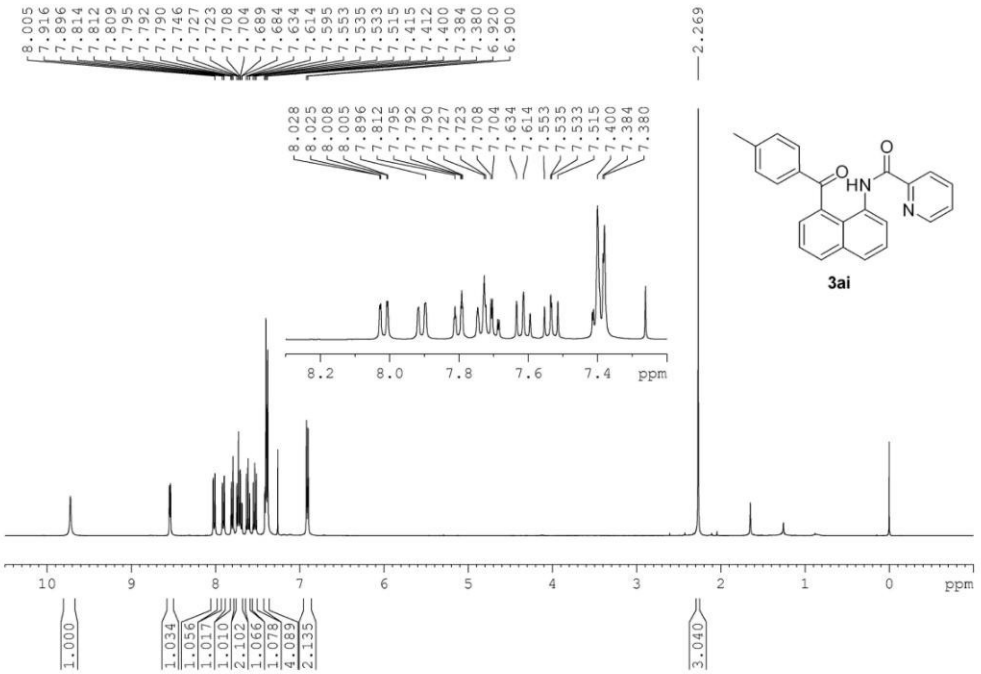
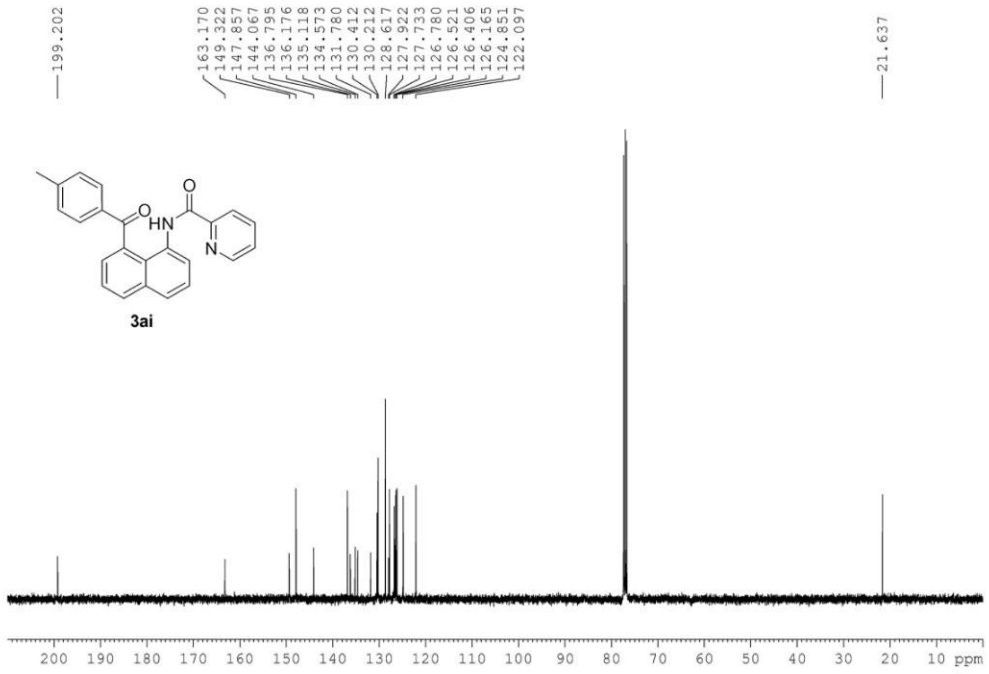
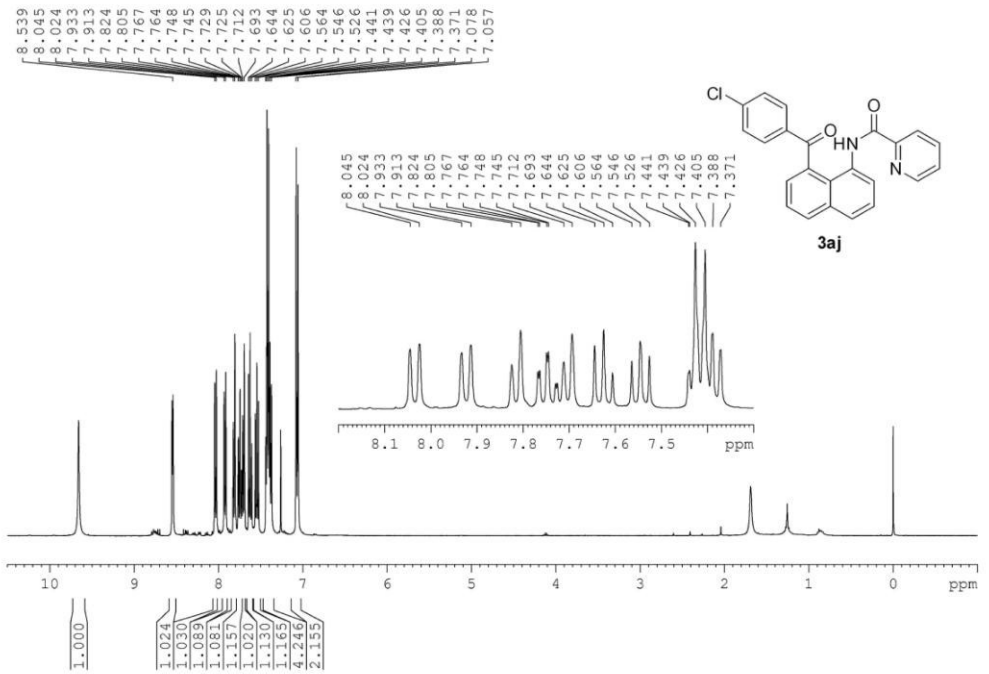
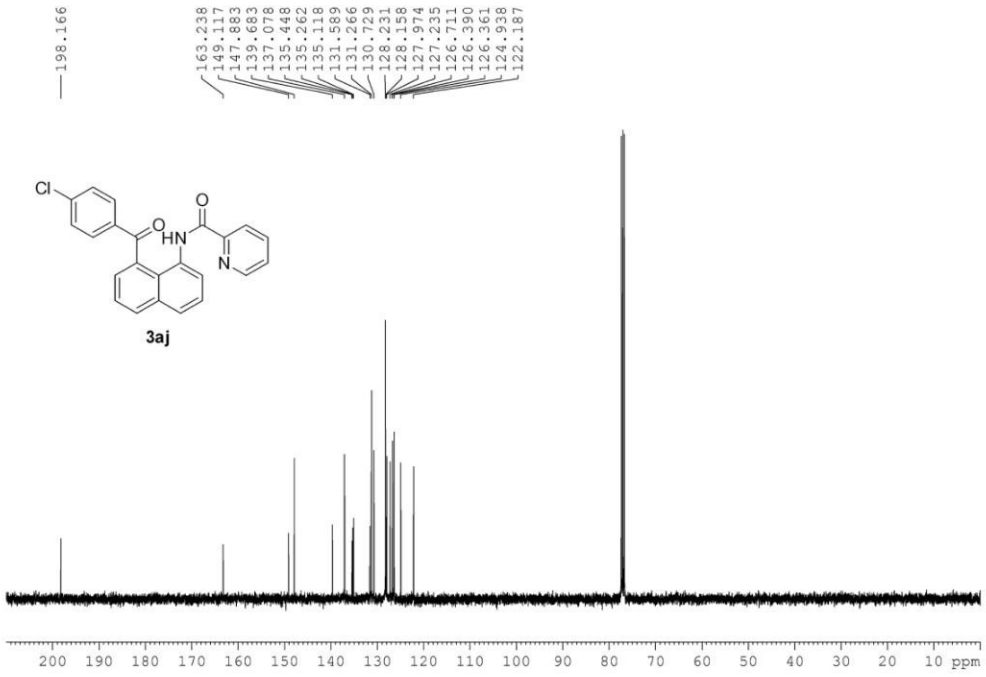
7.741
7.721
7.717
7.701
7.697
7.682
7.678
7.641
7.622
7.603
7.565
7.547
7.527
7.498
7.480
7.477
7.418
7.415
7.411
7.408
7.398
7.392
7.389
7.380
7.377
7.366
7.348
7.329
7.138
7.119
7.099
3ah
8.0 7.8 7.6 7.4 7.2 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.036
1.023
1.019
1.046
2.126
1.046
1.055
1.947
3.107
2.045

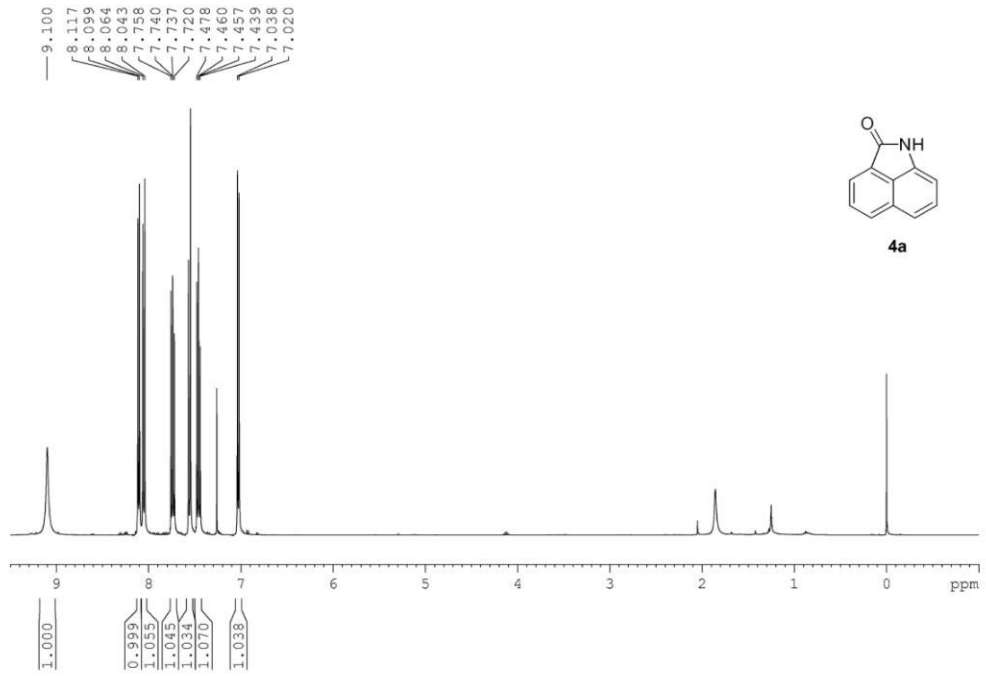

199.434
163.139
149.211
147.855
136.970
136.926
135.882
135.096
133.167
131.743
130.540
129.996
128.027
127.939
127.764
126.873
126.601
126.486
126.194
124.894
122.115
3ah
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

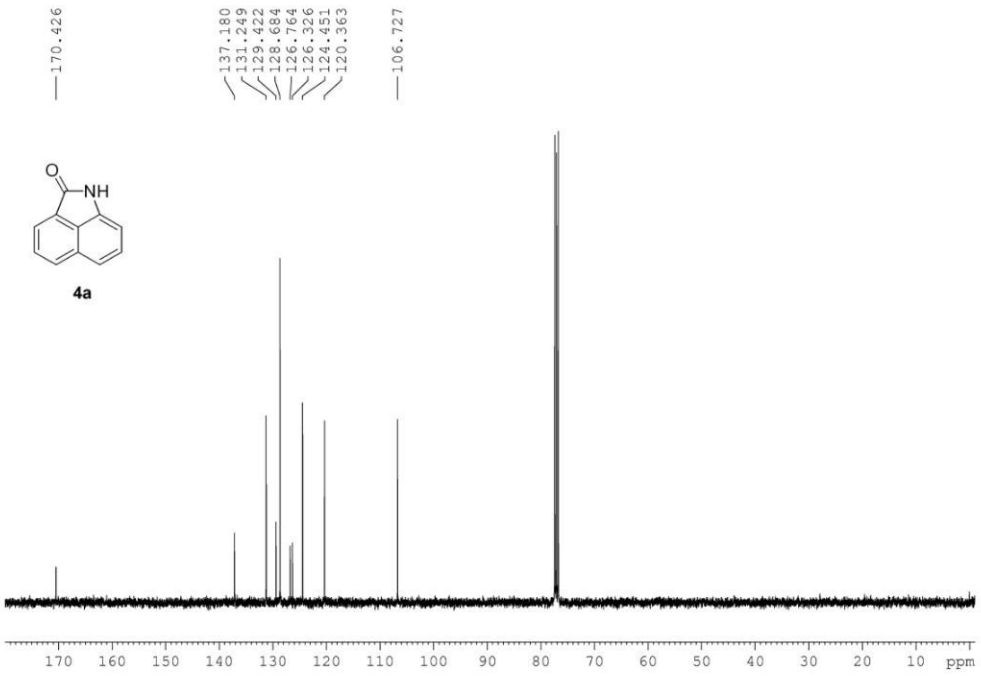

8.005
7.916
7.896
7.814
7.812
7.809
7.795
7.792
7.790
7.746
7.727
7.723
7.708
7.704
7.689
7.684
7.634
7.614
7.595
7.553
7.535
7.533
7.515
7.415
7.412
7.400
7.384
7.380
6.920
6.900
2.269
8.028
8.025
8.008
8.005
7.896
7.812
7.795
7.792
7.790
7.727
7.723
7.708
7.704
7.634
7.614
7.553
7.535
7.533
7.515
7.400
7.384
7.380
3ai
8.2 8.0 7.8 7.6 7.4 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.034
1.056
1.017
1.010
2.102
1.066
1.078
4.089
2.135
3.040

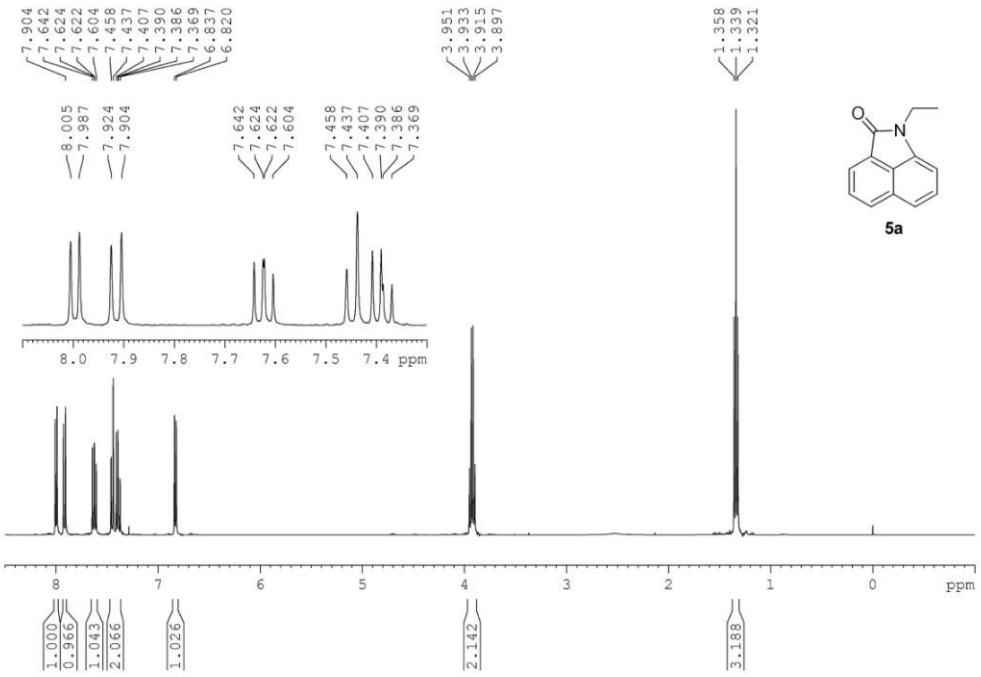

199.202
163.170
149.322
147.857
144.067
136.795
136.176
135.118
134.573
131.780
130.412
130.212
128.617
127.922
127.733
126.780
126.521
126.406
126.165
124.851
122.097
21.637
O
HN
O
N
3ai
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

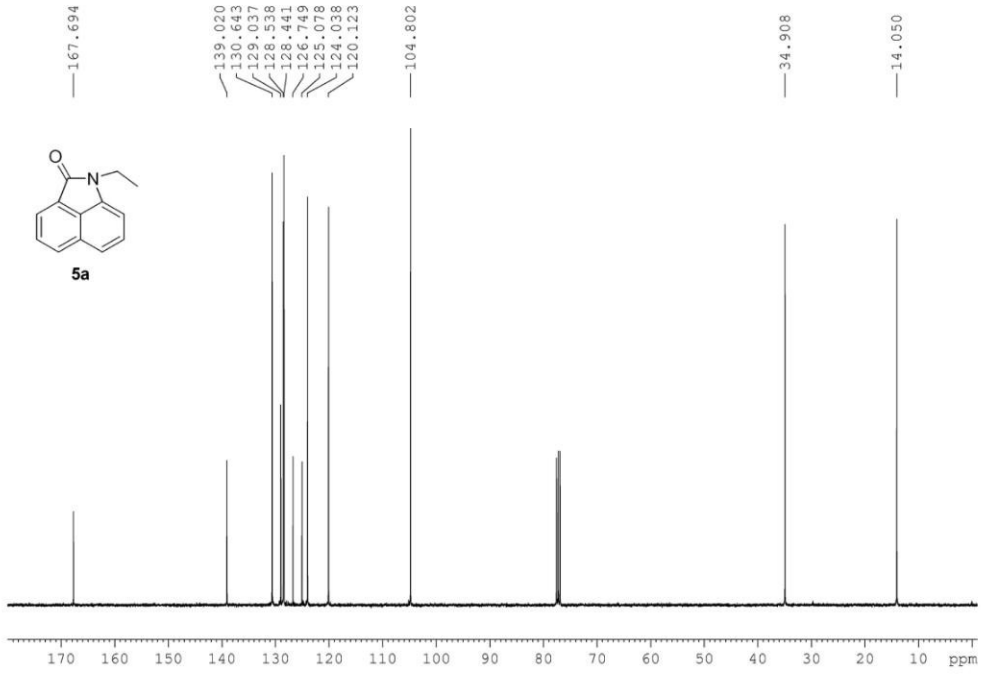

8.539
8.045
8.024
7.933
7.913
7.824
7.805
7.767
7.764
7.748
7.745
7.729
7.725
7.712
7.693
7.644
7.625
7.606
7.564
7.546
7.526
7.441
7.439
7.426
7.405
7.388
7.371
7.078
7.057
Cl
O
HN
O
N
3aj
8.1 8.0 7.9 7.8 7.7 7.6 7.5 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.024
1.030
1.089
1.081
1.157
1.020
1.130
1.165
4.246
2.155

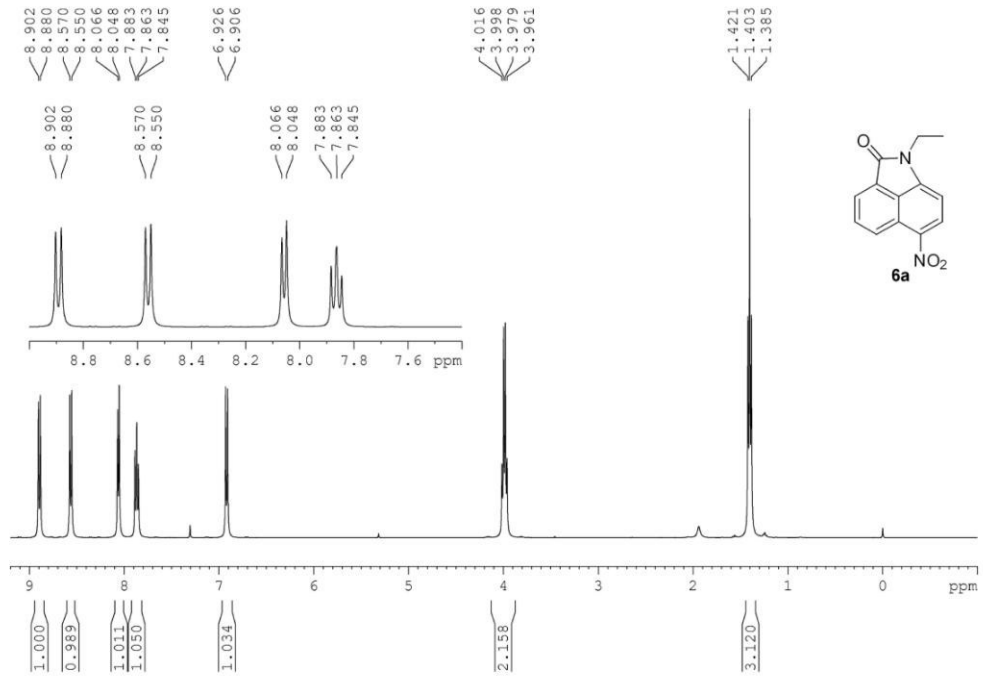

198.166
163.238
149.117
147.883
139.683
137.078
135.448
135.262
135.118
131.589
131.266
130.729
128.231
128.158
127.974
127.235
126.711
126.390
126.361
124.938
122.187
Cl
O
HN
O
N
3aj
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

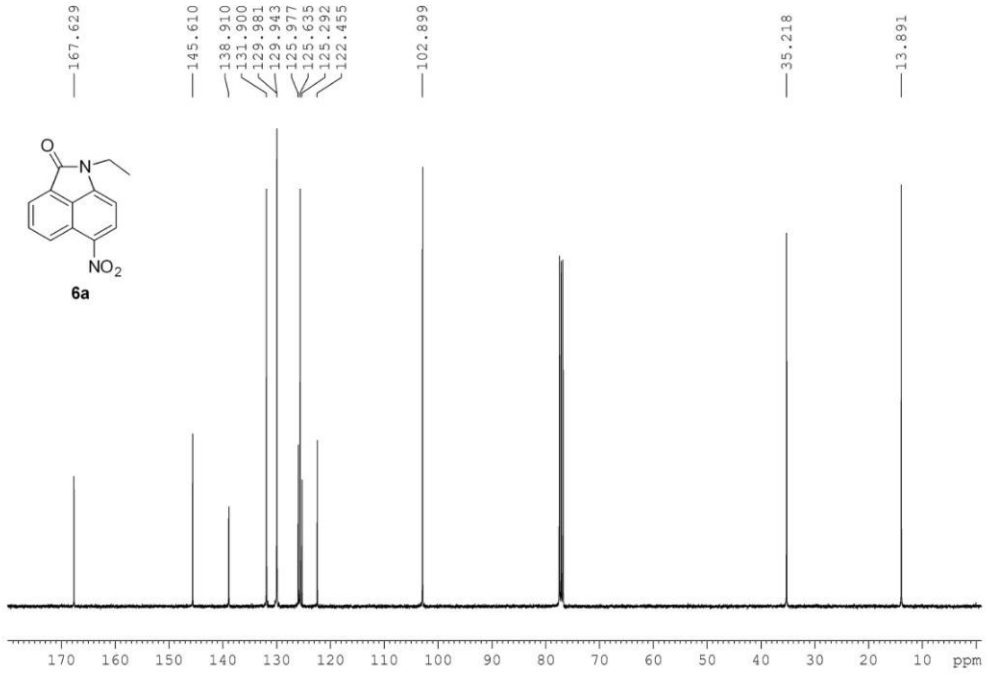

9.100
8.117
8.099
8.064
8.043
7.758
7.740
7.737
7.720
7.478
7.460
7.457
7.439
7.038
7.020
O
NH
4a
9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.999
1.055
1.045
1.034
1.070
1.038

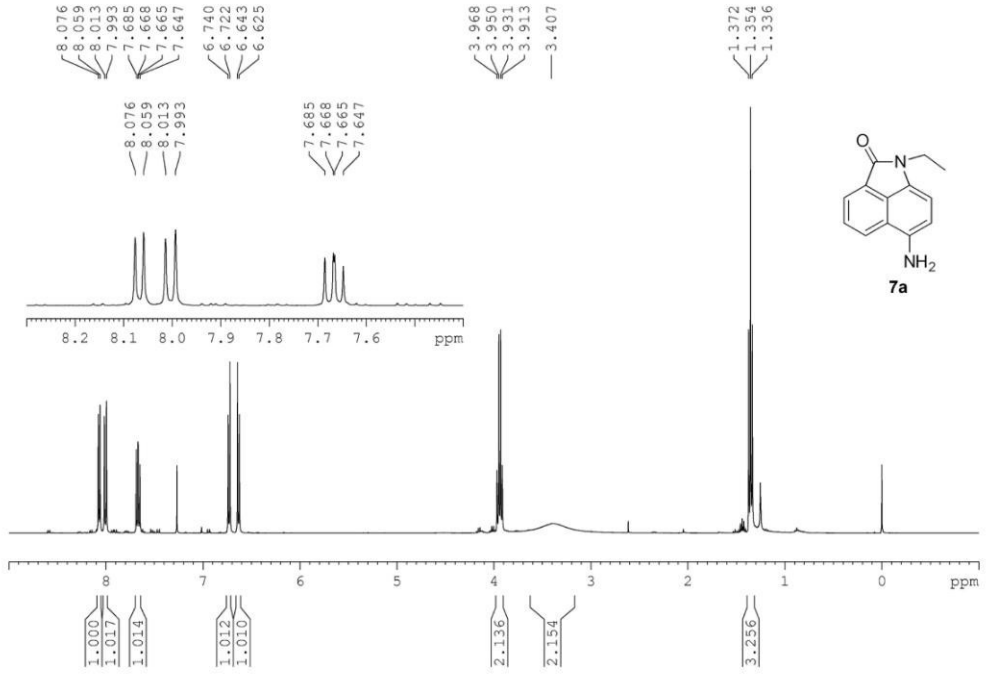

170.426
137.180
131.249
129.422
128.684
126.764
126.326
124.451
120.363
106.727
O
NH
4a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

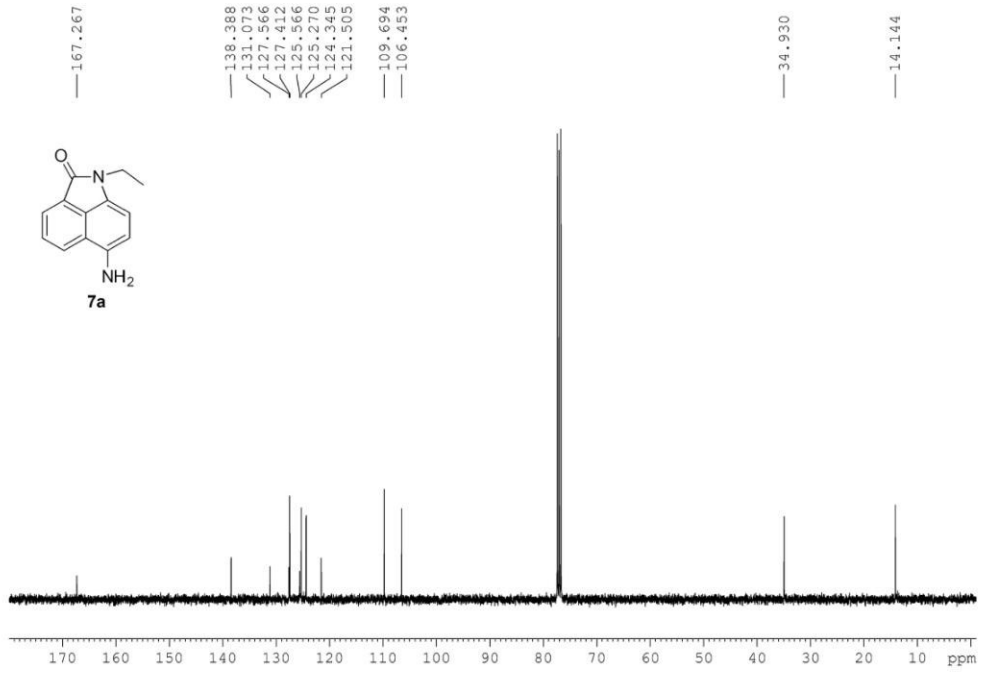

7.904
7.642
7.624
7.622
7.604
7.458
7.437
7.407
7.390
7.386
7.369
6.837
6.820
3.951
3.933
3.915
3.897
1.358
1.339
1.321
8.005
7.987
7.924
7.904
7.642
7.624
7.622
7.604
7.458
7.437
7.407
7.390
7.386
7.369
O
N
5a
8.0 7.9 7.8 7.7 7.6 7.5 7.4 ppm
8 7 6 5 4 3 2 1 0 ppm
1.000
0.966
1.043
2.066
1.026
2.142
3.188

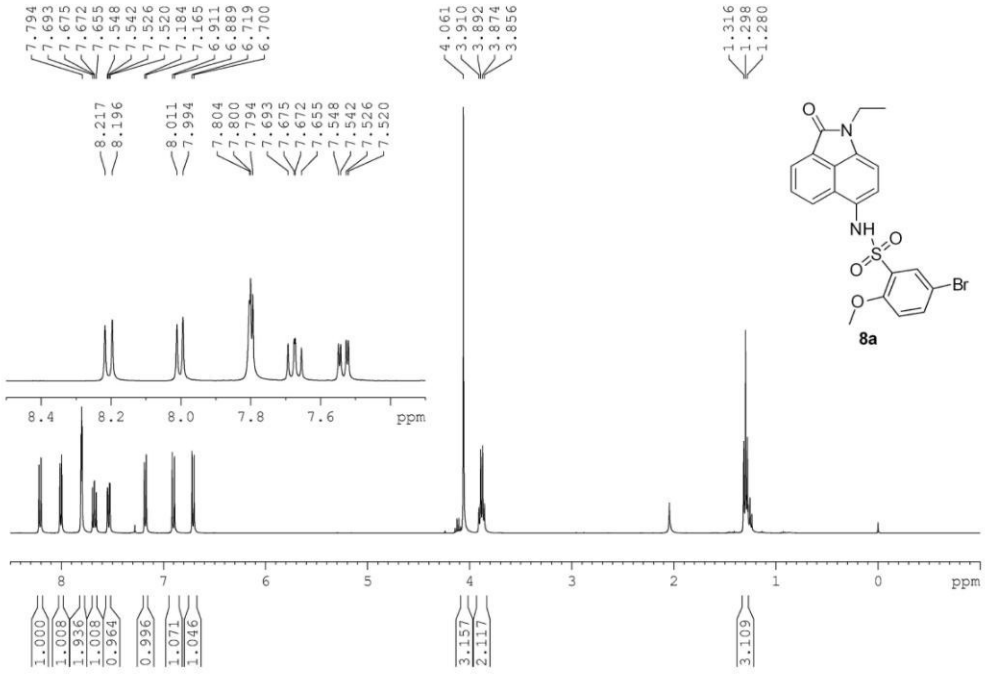

167.694
139.020
130.643
129.037
128.538
128.441
126.749
125.078
124.038
120.123
104.802
34.908
14.050
5a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

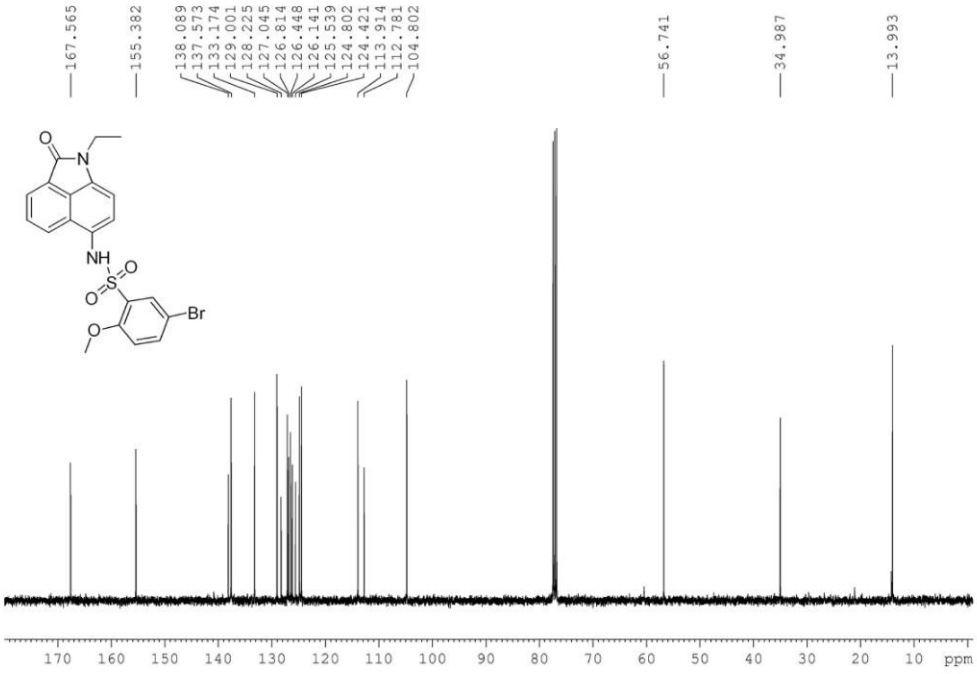

8.902
8.880
8.570
8.550
8.066
8.048
7.883
7.863
7.845
6.926
6.906
4.016
3.998
3.979
3.961
1.421
1.403
1.385
6a
8.8 8.6 8.4 8.2 8.0 7.8 7.6 ppm
9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.989
1.011
1.050
1.034
2.158
3.120


167.629
145.610
138.910
131.900
129.981
129.943
125.977
125.635
125.292
122.455
102.899
35.218
13.891
O
N
NO2
6a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.076
8.059
8.013
7.993
7.685
7.668
7.665
7.647
6.740
6.722
6.643
6.625
3.968
3.950
3.931
3.913
3.407
1.372
1.354
1.336
O
N
NH2
7a
8.2 8.1 8.0 7.9 7.8 7.7 7.6 ppm
8 7 6 5 4 3 2 1 0 ppm
1.000
1.017
1.014
1.012
1.010
2.136
2.154
3.256


167.267
138.388
131.073
127.566
127.412
125.566
125.270
124.345
121.505
109.694
106.453
34.930
14.144
O
N
NH2
7a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.794
7.693
7.675
7.672
7.655
7.548
7.542
7.526
7.520
7.184
7.165
6.911
6.889
6.719
6.700
8.217
8.196
8.011
7.994
7.804
7.800
7.794
7.693
7.675
7.672
7.655
7.548
7.542
7.526
7.520
4.061
3.910
3.892
3.874
3.856
1.316
1.298
1.280
O
N
NH
S
O
O
Br
O
8a
8.4 8.2 8.0 7.8 7.6 ppm
8 7 6 5 4 3 2 1 0 ppm
1.000
1.008
1.936
1.008
0.964
0.996
1.071
1.046
3.157
2.117
3.109


167.565
155.382
138.089
137.573
133.174
129.001
128.225
127.045
126.814
126.448
126.141
125.539
124.802
124.421
113.914
112.781
104.802
56.741
34.987
13.993
O
N
NH
O
S
O
Br
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm